

**STIC-EIC1800/2900**

*288329*

**From:** SEAN BASQUILL [sean.basquill@uspto.gov]  
**Sent:** Friday, March 06, 2009 10:48 AM  
**To:** STIC-EIC1800/2900  
**Subject:** Search Request, Case/Application No.: 10560012

**Requester:** SEAN BASQUILL (P/1612)  
**Art Unit:** GROUP ART UNIT 1612

**Case/Application number:** 10560012

**Priority Filing Date:** 10 June 2003

**Format for Search Results:** Email

**Meaning of unusual acronyms or initialisms:**

**Identify the novelty:**

Claim 29, as attached, recites approximately four-and-a-half pages of discrete chemical compound names of species within a genus as claimed. I would like to know if any of the compounds were known in the art prior to June 10, 2003.

**Additional comments:**

ONLY the chemical compounds as recited in Claim 29 (which yes, goes on for five pages) are of concern here.

**Attachment:** Yes (10560012 Claim 29.pdf)

*MG*  
3/6/2009

=> file registry  
FILE 'REGISTRY' ENTERED AT 11:02:00 ON 12 MAR 2009  
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10/560012

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STRUCTURE FILE UPDATES: 11 MAR 2009 HIGHEST RN 1119363-64-2

DICTIONARY FILE UPDATES: 11 MAR 2009 HIGHEST RN 1119363-64-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

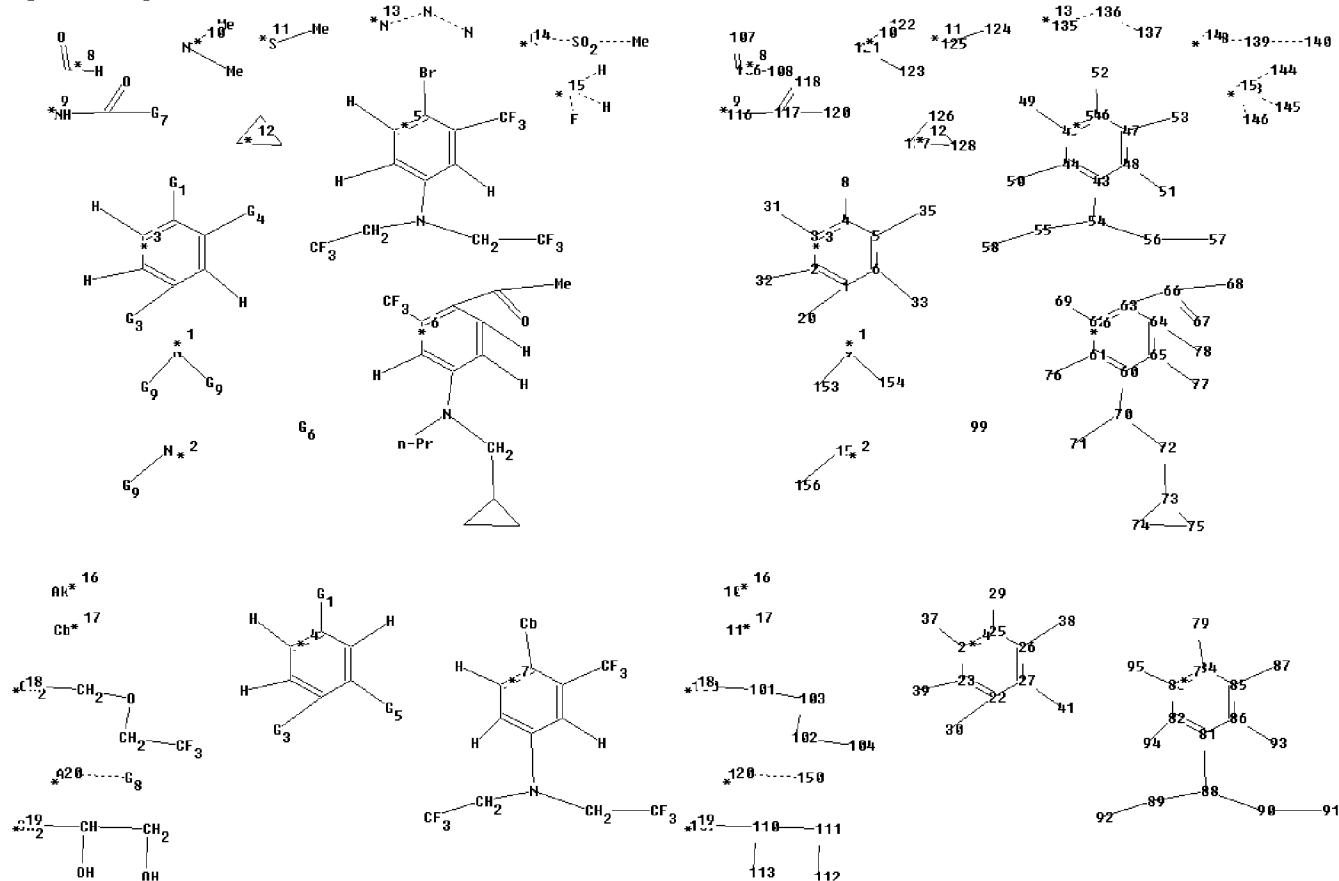
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

Uploading L26.str



10/560012

1 2 3 4 5 6 22 23 24 25 26 27 43 44 45 46 47 48 60 61 62 63  
64 65 73 74 75 81 82 83 84 85 86 126 127 128

chain bonds :

1-20 2-32 3-31 4-8 5-35 6-33 9-153 9-154 15-156 22-30 23-39 24-37 25-29  
26-38 27-41 43-54 44-50 45-49 46-52 47-53 48-51 54-55 54-56 55-58 56-57  
60-70 61-76  
62-69 63-66 64-78 65-77 66-67 66-68 70-71 70-72 72-73 79-84 81-88 82-94  
83-95 85-87  
86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-108  
106-107 109-110  
110-111 110-113 111-112 115-150 116-117 117-118 117-120 121-122 121-123  
124-125 135-136  
136-137 138-139 139-140 143-144 143-145 143-146

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-  
48  
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 73-74 73-75  
74-75 81-82  
81-86 82-83 83-84 84-85 85-86 126-127 126-128 127-128

exact/norm bonds :

1-20 4-8 5-35 9-153 9-154 15-156 22-30 25-29 27-41 43-54 60-70 66-67  
73-74 73-75 74-75 81-88 106-107 110-113 115-150 116-117 117-118 117-120  
126-127 126-128  
127-128 135-136 136-137 138-139 139-140 143-144 143-145 143-146

exact bonds :

2-32 3-31 6-33 23-39 24-37 26-38 44-50 45-49 46-52 47-53 48-51 54-55  
54-56 55-58 56-57 61-76 62-69 63-66 64-78 65-77 66-68 70-71 70-72 72-73  
79-84 82-94 83-95  
85-87 86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-  
108 109-110  
110-111 111-112 121-122 121-123 124-125

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-  
48  
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 81-82 81-86  
82-83 83-84  
84-85 85-86

isolated ring systems :

containing 1 : 22 : 43 : 60 : 81 :

G1:CN,NO2

G3:[\*1],[\*2]

G4:CF3,C1,NO2,CH3,OH,CN

G5:CH3,CF3,NO2,C1

G6:[\*3],[\*4],[\*5],[\*6],[\*7]

G7:CH3,MeO,t-BuO

G8:CF3,OH,MeO,EtO,NH2,[\*8],[\*9],[\*10],[\*11],[\*12],[\*13],[\*14],[\*15]

G9:[\*16],[\*17],[\*18],[\*19],[\*20]

Hydrogen count :

9:= exact 0 15:= exact 1

Connectivity :

10/560012

9:3 E exact RC ring/chain 10:1 E exact RC ring/chain 11:1 E exact RC ring/chain  
15:2 E exact RC ring/chain 79:1 E exact RC ring/chain 115:2 E exact RC ring/chain  
125:2 E exact  
RC ring/chain 126:2 E exact RC ring/chain 128:2 E exact RC ring/chain 138:2 E  
exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom  
15:CLASS 20:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 29:CLASS  
30:CLASS 31:CLASS  
32:CLASS 33:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 41:CLASS 43:Atom  
44:Atom 45:Atom  
46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS  
54:CLASS 55:CLASS  
56:CLASS 57:CLASS 58:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom  
66:CLASS  
67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:Atom 74:Atom  
75:Atom 76:CLASS 77:CLASS  
78:CLASS 79:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:CLASS  
88:CLASS  
89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 95:CLASS 99:CLASS  
100:CLASS 101:CLASS  
102:CLASS 103:CLASS 104:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS  
110:CLASS 111:CLASS  
112:CLASS 113:CLASS 115:CLASS 116:CLASS 117:CLASS 118:CLASS 120:CLASS  
121:CLASS 122:CLASS  
123:CLASS 124:CLASS 125:CLASS 126:Atom 127:Atom 128:Atom 135:CLASS 136:CLASS  
137:CLASS  
138:CLASS 139:CLASS 140:CLASS 143:CLASS 144:CLASS 145:CLASS 146:CLASS  
150:CLASS 153:CLASS  
154:CLASS 156:CLASS

Generic attributes :

11:  
Saturation : Saturated  
79:  
Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Type of Ring System : Monocyclic

Element Count :

Node 10: Limited  
C,C7

Node 11: Limited  
C,C6

Node 79: Limited  
C,C6

Node 115: Limited  
C,C6

=> file zcaplus  
FILE 'ZCAPLUS' ENTERED AT 11:02:04 ON 12 MAR 2009  
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FILE COVERS 1907 - 12 Mar 2009 VOL 150 ISS 11  
FILE LAST UPDATED: 11 Mar 2009 (20090311/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

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10/560012

L14 SCR 616  
L26 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L27 SCR 1993  
L32 SCR 1840 OR 2043 OR 1951  
L35 898352 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (N>1 AND ((46.150.18/RID AND 1/NRS) OR (46.150.18/RID AND (1.13.1/RID OR 16.127.1/RID OR 46.150.1/RID) AND 2/NRS))) NOT PMS/CI  
L38 1054 SEA FILE=REGISTRY SUB=L35 SSS FUL L26 AND ((L14 AND L27) NOT L32)  
L47 135 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L38 AND L3  
L48 16 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L3 NOT L47  
L50 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L48 AND BR/ELS AND 9/F  
L51 10 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L48 NOT BR/ELS  
L52 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L51 AND F/ELS  
L53 7 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L50 OR L52  
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L55 65815 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (C14H19N3O2/MF OR C13H17N3O2/MF OR C12H13F3N2/MF OR C13H12F6N20/MF OR C13H13N3O2/MF OR C15H19F3N2/MF OR C11H11F3N202/MF OR C11H8F6N2/MF OR C12H11F3N2/MF OR C13H15F3N2/MF OR C13H15N3O2/MF OR C13H16N202/MF OR C13H17CLN2/MF OR C13H17N3O3/MF OR C13H20N202/MF OR C14H14F6N2/MF OR C14H15F3N20/MF OR C14H17F3N2/MF OR C14H17F3N202/MF OR C14H17N3O2/MF OR C15H17F3N2/MF OR C15H17F3N20/MF OR C15H17F3N202/MF OR C16H17F3N2/MF OR C16H21F3N2/MF OR C10H11F3N202/MF OR C10H11F3N203/MF OR C10H13CLN203/MF OR C10H6F6N2/MF OR C10H9F3N2/MF OR C11H11F3N2/MF OR C11H11F3N20/MF OR C11H13F3N202/MF OR C11H13F3N203/MF OR C11H13N3O3/MF OR C11H15CLN202/MF OR C11H16CLN302/MF OR C11H16N203/MF OR C11H7BRF9N/MF OR C12H10F6N2/MF OR C12H10F6N20/MF OR C12H11F5N2/MF OR C12H11F6N3/MF OR C12H13F3N20/MF OR C12H16CLN3/MF OR C12H18CLN302/MF OR C12H18N203/MF OR C12H7F9N2/MF OR C12H8F8N2/MF OR C12H9F6N5/MF OR C12H9F7N2/MF OR C13H12F6N2/MF OR C13H12F6N203/S/MF OR C13H12F6N2S/MF OR C13H13CLN2/MF OR C13H13F3N2/MF OR C13H13F3N202/MF OR C13H13F6N3O2S/MF OR C13H15CLN2/MF OR C13H15F3N202/MF OR C13H15F3N203/MF OR C13H17CLN20/MF OR C13H17F3N202/MF OR C13H17F3N203/MF OR C13H17F3N204/MF OR C13H18N203/MF OR C13H20N203/MF OR C13H8F6N2/MF OR C14H11F9N20/MF OR C14H12F6N2/MF OR C14H13F3N2/MF OR C14H13F6N30/MF OR C14H13F6N302/MF OR C14H14F6N20/MF OR C14H15F3N2/MF OR C14H17CLN2/MF OR C14H17F3N20/MF OR C14H17F3N203/MF OR C14H20N202/MF OR C14H22N202/MF OR C15H14F6N2/MF OR C15H16F6N2/MF OR C15H17F3N202/MF OR C15H19N3O2/MF OR C15H21CLN2/MF OR C15H21F3N202/MF OR C15H21N3O2/MF OR C15H24N202/MF OR C16H19F3N2/MF OR C16H19F3N202/MF OR C16H20F3NO/MF OR C16H21F3N20/MF OR C16H21F3N202/MF OR C17H12F9N/MF OR C17H19F6N3O2/MF OR C17H23F3N2/MF OR C17H25N3O2/MF OR C18H27F3N4/MF OR C21H31F3N20SI/MF OR C9H6F6N202/MF)  
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L66 142 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L55 AND L54  
L67 366 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L56 OR L66  
L68 68 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L67  
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10/560012

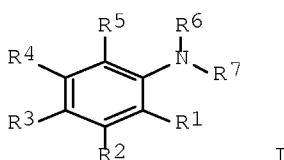
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L69 ANSWER 1 OF 1 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2005:14359 ZCPLUS Full-text  
DOCUMENT NUMBER: 142:113710  
TITLE: Preparation of substituted anilines as androgen receptor modulators  
INVENTOR(S): Blanc, Jean-Baptiste E.; Cadilla, Rodolfo; Cowan, David John; Kaldor, Istvan; Larkin, Andrew L.; Stewart, Eugene Lee; Turnbull, Philip Stewart; Trump, Ryan Paul  
PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA  
SOURCE: PCT Int. Appl., 86 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005000795	A2	20050106	WO 2004-US18252	20040609
WO 2005000795	A3	20050310		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1654221	A2	20060510	EP 2004-776383	20040609
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR			
JP 2007500245	T	20070111	JP 2006-533629	20040609
US 20060148893	A1	20060706	US 2005-560012	20051208 <--
PRIORITY APPLN. INFO.:			US 2003-477252P	P 20030610
			WO 2004-US18252	W 20040609

OTHER SOURCE(S): MARPAT 142:113710

GI



AB This invention relates to non-steroidal compds. I [R1, R2, R4, R5 = H, CN, NO<sub>2</sub>, halo, etc. (at least one of R1, R2, R4, R5 is not H); R3 = CN, NO<sub>2</sub>, halo, etc.; R6, R7 = H, (Ra)<sub>x</sub>R9 (Ra = alkylene; x = 0-1; R9 = alkyl, haloalkyl,

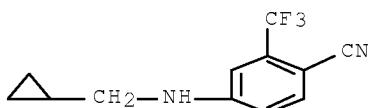
hydroxyalkyl, etc.)] that are or are believed to be modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, and also to the methods for the making and use of such compds. Thus, reacting 4-fluoro-2-trifluoromethylbenzonitrile with N-(cyclopropylmethyl)-N-propylamine afforded 81% I [R1, R2, R5 = H; R3 = CN; R4 = CF<sub>3</sub>; R6 = CH<sub>2</sub>(cyclopropyl); R7 = Pr]. The compds. I are claimed to be useful in the treatment or prophylaxis of conditions or disorders that respond to selective androgen receptor modulation (no data given). The pharmaceutical composition comprising the compound I is disclosed.

IT 821777-24-6P 821777-27-9P 821777-32-6P  
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 821777-38-2P 821777-41-7P 821777-42-8P  
 821777-44-0P 821777-50-8P 821777-58-6P  
 821777-66-6P 821777-68-8P 821777-73-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of substituted anilines as androgen receptor modulators)

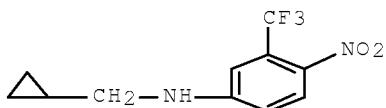
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CN Benzonitrile, 4-[(cyclopropylmethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



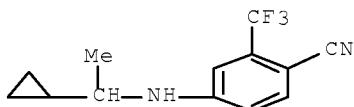
RN 821777-27-9 ZCPLUS

CN Benzenamine, N-(cyclopropylmethyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-32-6 ZCPLUS

CN Benzonitrile, 4-[(1-cyclopropylethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

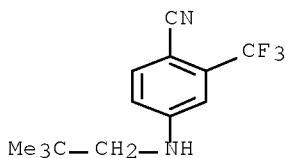


RN 821777-34-8 ZCPLUS

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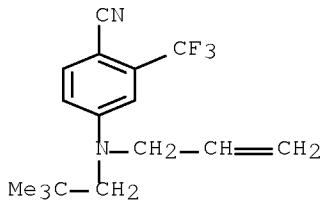
10/560012

INDEX NAME)



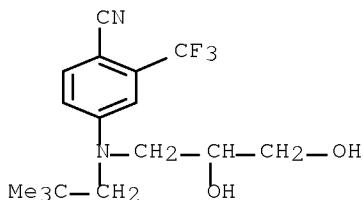
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CN Benzonitrile, 4-[(2,2-dimethylpropyl)-2-propen-1-ylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



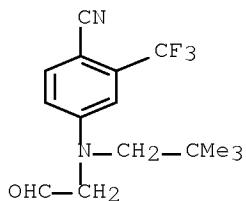
RN 821777-37-1 ZCPLUS

CN Benzonitrile, 4-[(2,3-dihydroxypropyl)(2,2-dimethylpropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



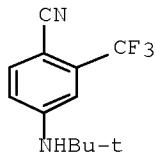
RN 821777-38-2 ZCPLUS

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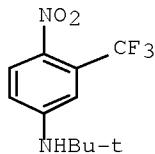


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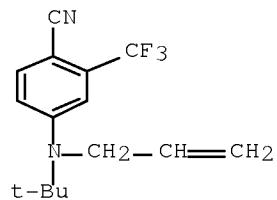
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CN Benzonitrile, 4-[(1,1-dimethylethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



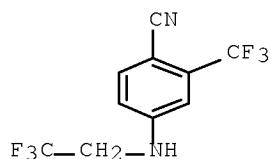
RN 821777-42-8 ZCPLUS  
CN Benzenamine, N-(1,1-dimethylethyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-44-0 ZCPLUS  
CN Benzonitrile, 4-[(1,1-dimethylethyl)-2-propen-1-ylamino]-2-(trifluoromethyl)- (CA INDEX NAME)

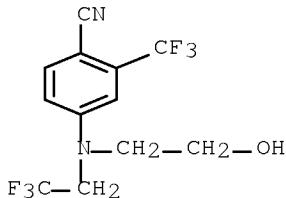


RN 821777-50-8 ZCPLUS  
CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

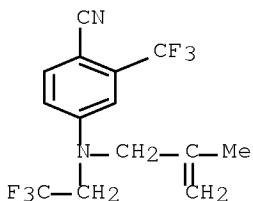


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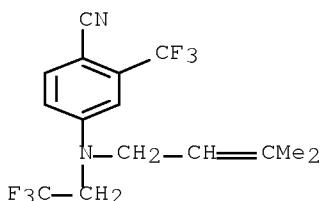
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CN Benzonitrile, 4-[(2-hydroxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



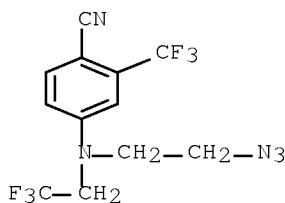
RN 821777-66-6 ZCPLUS  
CN Benzonitrile, 4-[(2-methyl-2-propen-1-yl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-68-8 ZCPLUS  
CN Benzonitrile, 4-[(3-methyl-2-buten-1-yl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-73-5 ZCPLUS  
CN Benzonitrile, 4-[(2-azidoethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



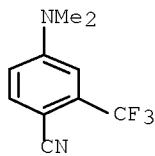
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 821776-49-2P 821776-50-5P 821776-51-6P  
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 821777-74-6P 821777-75-7P 821777-76-8P  
 821777-77-9P 821777-78-0P 821778-33-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

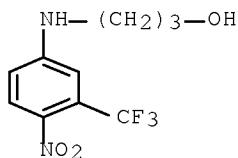
(preparation of substituted anilines as androgen receptor modulators)

RN 51332-25-3 ZCPLUS

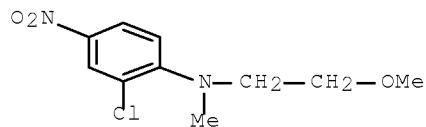
CN Benzonitrile, 4-(dimethylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



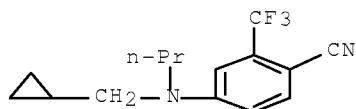
RN 115416-50-7 ZCPLUS  
 CN 1-Propanol, 3-[(4-nitro-3-(trifluoromethyl)phenyl)amino]- (CA INDEX NAME)



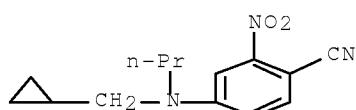
RN 151951-35-8 ZCPLUS  
 CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



RN 821776-43-6 ZCPLUS  
 CN Benzonitrile, 4-[(cyclopropylmethyl)propylamino]-2-(trifluoromethyl)- (CA INDEX NAME)

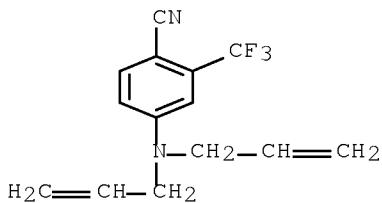


RN 821776-44-7 ZCPLUS  
 CN Benzonitrile, 4-[(cyclopropylmethyl)propylamino]-2-nitro- (CA INDEX NAME)

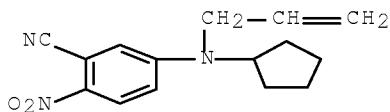


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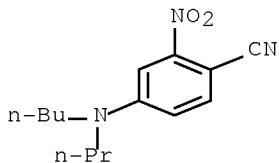
RN 821776-45-8 ZCPLUS  
CN Benzonitrile, 4-(di-2-propen-1-ylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



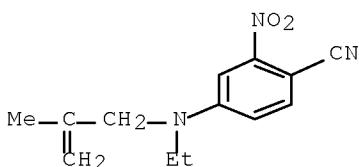
RN 821776-46-9 ZCPLUS  
CN Benzonitrile, 5-(cyclopentyl-2-propen-1-ylamino)-2-nitro- (CA INDEX NAME)



RN 821776-47-0 ZCPLUS  
CN Benzonitrile, 4-(butylpropylamino)-2-nitro- (CA INDEX NAME)



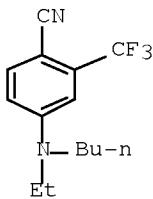
RN 821776-48-1 ZCPLUS  
CN Benzonitrile, 4-[ethyl(2-methyl-2-propen-1-yl)amino]-2-nitro- (CA INDEX NAME)



10/560012

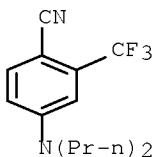
RN 821776-49-2 ZCPLUS

CN Benzonitrile, 4-(butylethylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



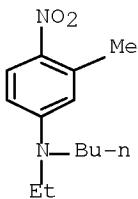
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CN Benzonitrile, 4-(dipropylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



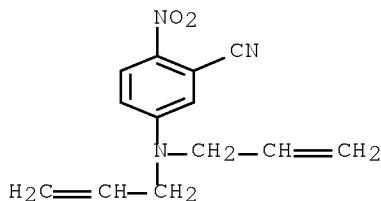
RN 821776-51-6 ZCPLUS

CN Benzenamine, N-butyl-N-ethyl-3-methyl-4-nitro- (CA INDEX NAME)



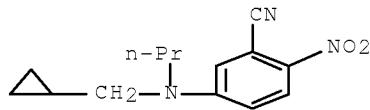
RN 821776-52-7 ZCPLUS

CN Benzonitrile, 5-(di-2-propen-1-ylamino)-2-nitro- (CA INDEX NAME)

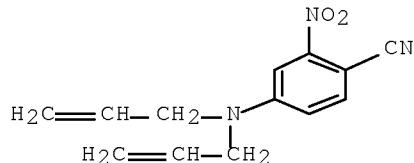


10/560012

RN 821776-53-8 ZCPLUS  
CN Benzonitrile, 5-[(cyclopropylmethyl)propylamino]-2-nitro- (CA INDEX NAME)



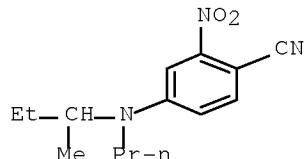
RN 821776-54-9 ZCPLUS  
CN Benzonitrile, 4-(di-2-propen-1-ylamino)-2-nitro- (CA INDEX NAME)



RN 821776-55-0 ZCPLUS  
CN Benzenamine, 3-methyl-4-nitro-N,N-dipropyl- (CA INDEX NAME)

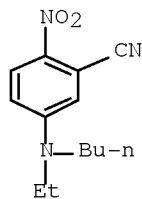


RN 821776-56-1 ZCPLUS  
CN Benzonitrile, 4-[(1-methylpropyl)propylamino]-2-nitro- (CA INDEX NAME)

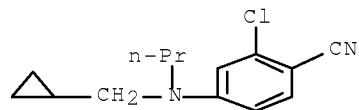


RN 821776-57-2 ZCPLUS  
CN Benzonitrile, 5-(butylethylamino)-2-nitro- (CA INDEX NAME)

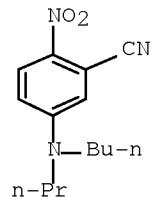
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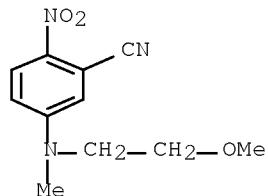
RN 821776-58-3 ZCPLUS  
CN Benzonitrile, 2-chloro-4-[ (cyclopropylmethyl)propylamino]- (CA INDEX NAME)



RN 821776-59-4 ZCPLUS  
CN Benzonitrile, 5-(butylpropylamino)-2-nitro- (CA INDEX NAME)

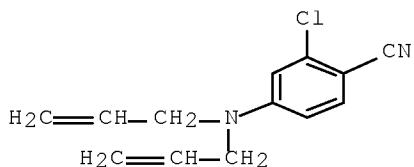


RN 821776-60-7 ZCPLUS  
CN Benzonitrile, 5-[ (2-methoxyethyl)methylamino]-2-nitro- (CA INDEX NAME)



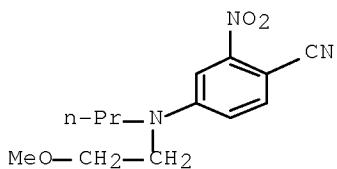
RN 821776-61-8 ZCPLUS  
CN Benzonitrile, 2-chloro-4-(di-2-propen-1-ylamino)- (CA INDEX NAME)

10/560012



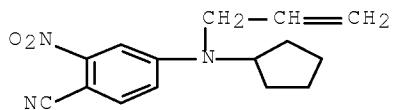
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CN Benzonitrile, 4-[(2-methoxyethyl)propylamino]-2-nitro- (CA INDEX NAME)



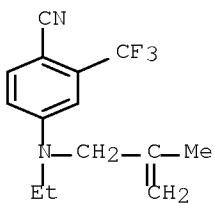
RN 821776-63-0 ZCPLUS

CN Benzonitrile, 4-(cyclopentyl-2-propen-1-ylamino)-2-nitro- (CA INDEX NAME)



RN 821776-64-1 ZCPLUS

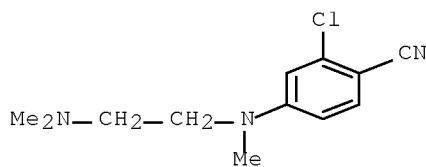
CN Benzonitrile, 4-[ethyl(2-methyl-2-propen-1-yl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-65-2 ZCPLUS

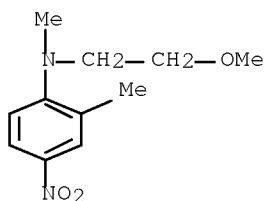
CN Benzonitrile, 2-chloro-4-[(2-(dimethylamino)ethyl)methylamino]- (CA INDEX NAME)

10/560012



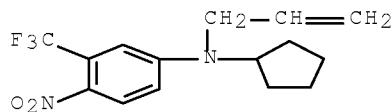
RN 821776-66-3 ZCPLUS

CN Benzenamine, N-(2-methoxyethyl)-N,2-dimethyl-4-nitro- (CA INDEX NAME)



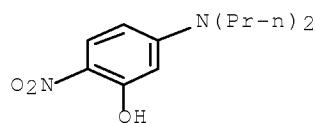
RN 821776-67-4 ZCPLUS

CN Benzenamine, N-cyclopentyl-4-nitro-N-2-propenyl-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-68-5 ZCPLUS

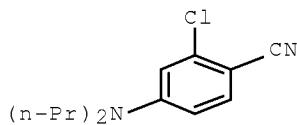
CN Phenol, 5-(dipropylamino)-2-nitro- (CA INDEX NAME)



RN 821776-69-6 ZCPLUS

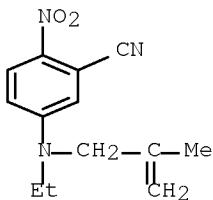
CN Benzonitrile, 2-chloro-4-(dipropylamino)- (CA INDEX NAME)

10/560012



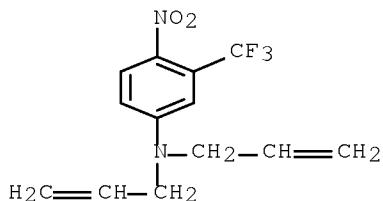
RN 821776-70-9 ZCPLUS

CN Benzonitrile, 5-[ethyl(2-methyl-2-propen-1-yl)amino]-2-nitro- (CA INDEX NAME)



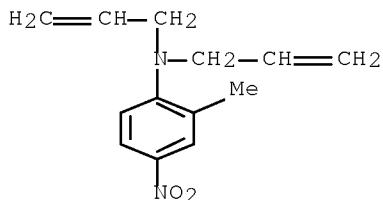
RN 821776-71-0 ZCPLUS

CN Benzenamine, 4-nitro-N,N-di-2-propen-1-yl-3-(trifluoromethyl)- (CA INDEX NAME)



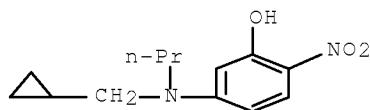
RN 821776-72-1 ZCPLUS

CN Benzenamine, 2-methyl-4-nitro-N,N-di-2-propen-1-yl- (CA INDEX NAME)

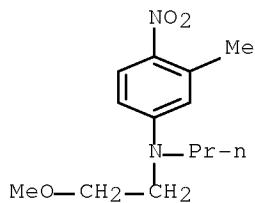


RN 821776-73-2 ZCPLUS

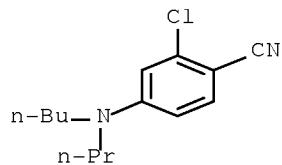
CN Phenol, 5-[(cyclopropylmethyl)propylamino]-2-nitro- (CA INDEX NAME)



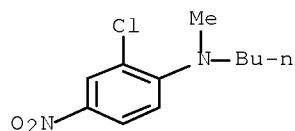
RN 821776-74-3 ZCPLUS  
CN Benzenamine, N-(2-methoxyethyl)-3-methyl-4-nitro-N-propyl- (CA INDEX NAME)



RN 821776-75-4 ZCPLUS  
CN Benzonitrile, 4-(butylpropylamino)-2-chloro- (CA INDEX NAME)

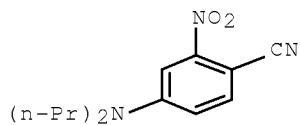


RN 821776-76-5 ZCPLUS  
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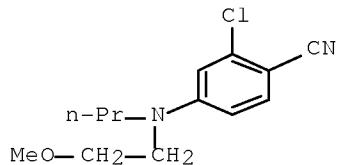
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CN Benzonitrile, 4-(dipropylamino)-2-nitro- (CA INDEX NAME)

10/560012



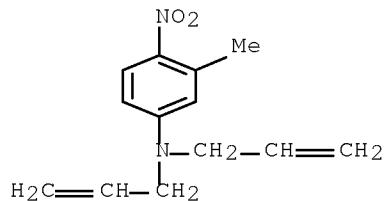
RN 821776-78-7 ZCPLUS

CN Benzonitrile, 2-chloro-4-[ (2-methoxyethyl)propylamino]- (CA INDEX NAME)



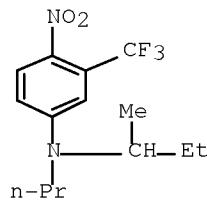
RN 821776-79-8 ZCPLUS

CN Benzenamine, 3-methyl-4-nitro-N,N-di-2-propen-1-yl- (CA INDEX NAME)



RN 821776-80-1 ZCPLUS

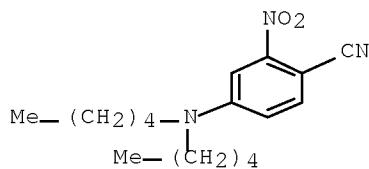
CN Benzenamine, N-(1-methylpropyl)-4-nitro-N-propyl-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-81-2 ZCPLUS

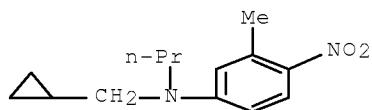
CN Benzonitrile, 4-(dipentylamino)-2-nitro- (CA INDEX NAME)

10/560012



RN 821776-82-3 ZCPLUS

CN Benzenamine, N-(cyclopropylmethyl)-3-methyl-4-nitro-N-propyl- (CA INDEX NAME)



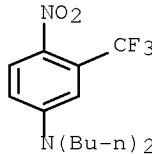
RN 821776-83-4 ZCPLUS

CN Benzonitrile, 5-(dipropylamino)-2-nitro- (CA INDEX NAME)



RN 821776-84-5 ZCPLUS

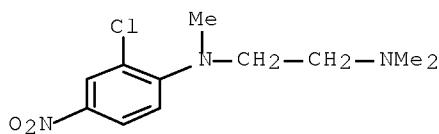
CN Benzenamine, N,N-dibutyl-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-85-6 ZCPLUS

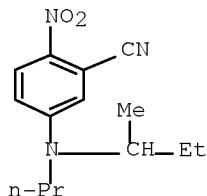
CN 1,2-Ethanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N2,N2-trimethyl- (CA INDEX NAME)

10/560012



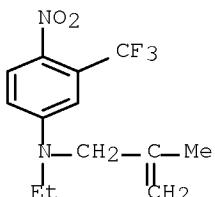
RN 821776-86-7 ZCPLUS

CN Benzonitrile, 5-[(1-methylpropyl)propylamino]-2-nitro- (CA INDEX NAME)



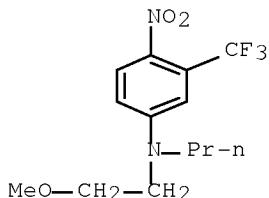
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CN Benzenamine, N-ethyl-N-(2-methyl-2-propenyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



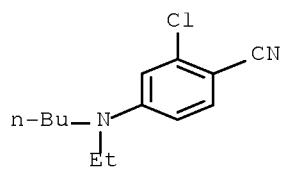
RN 821776-88-9 ZCPLUS

CN Benzenamine, N-(2-methoxyethyl)-4-nitro-N-propyl-3-(trifluoromethyl)- (CA INDEX NAME)

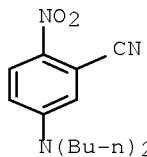


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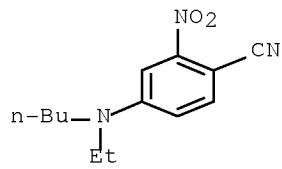
CN Benzonitrile, 4-(butylethylamino)-2-chloro- (CA INDEX NAME)



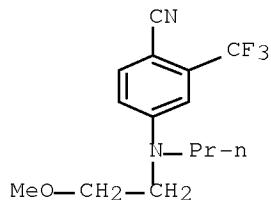
RN 821776-90-3 ZCPLUS  
 CN Benzonitrile, 5-(dibutylamino)-2-nitro- (CA INDEX NAME)



RN 821776-91-4 ZCPLUS  
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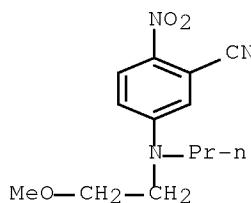


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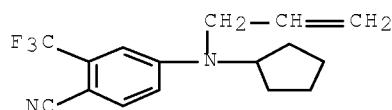


RN 821776-93-6 ZCPLUS  
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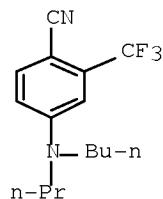
10/560012



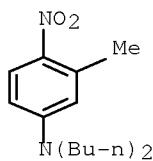
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CN Benzonitrile, 4-(cyclopentyl-2-propen-1-ylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-95-8 ZCPLUS  
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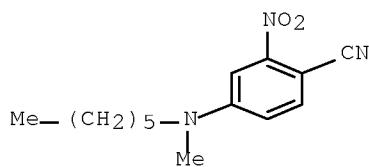


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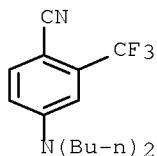
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CN Benzonitrile, 4-(hexylmethylamino)-2-nitro- (CA INDEX NAME)

10/560012



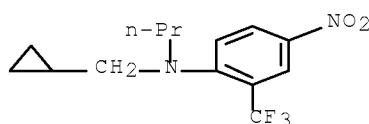
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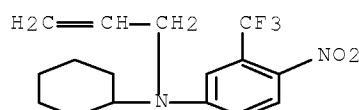
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RN 821777-00-8 ZCPLUS

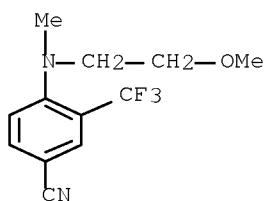
CN Benzenamine, N-cyclohexyl-4-nitro-2-propenyl-3-(trifluoromethyl)- (CA INDEX NAME)



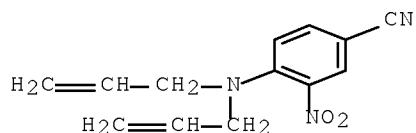
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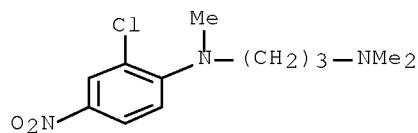
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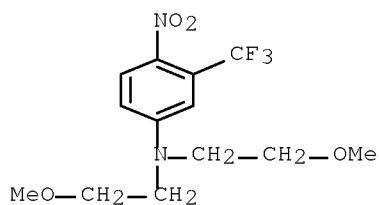
RN 821777-02-0 ZCPLUS  
CN Benzonitrile, 4-(di-2-propen-1-ylamino)-3-nitro- (CA INDEX NAME)



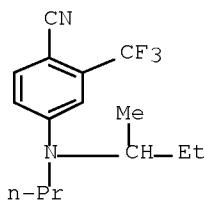
RN 821777-03-1 ZCPLUS  
CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



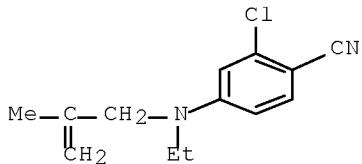
RN 821777-04-2 ZCPLUS  
CN Benzenamine, N,N-bis(2-methoxyethyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



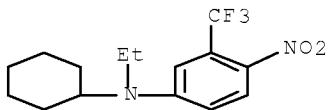
RN 821777-05-3 ZCPLUS  
CN Benzonitrile, 4-[1-(methylpropyl)propylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



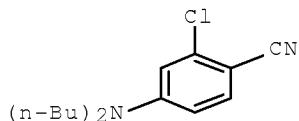
RN 821777-06-4 ZCPLUS  
 CN Benzonitrile, 2-chloro-4-[ethyl(2-methyl-2-propen-1-yl)amino]- (CA INDEX NAME)



RN 821777-07-5 ZCPLUS  
 CN Benzenamine, N-cyclohexyl-N-ethyl-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)

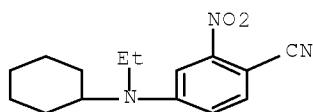


RN 821777-08-6 ZCPLUS  
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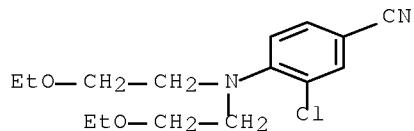
RN 821777-09-7 ZCPLUS  
 CN Benzonitrile, 4-(cyclohexylethylamino)-2-nitro- (CA INDEX NAME)

10/560012



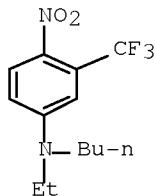
RN 821777-10-0 ZCPLUS

CN Benzonitrile, 4-[bis(2-ethoxyethyl)amino]-3-chloro- (CA INDEX NAME)



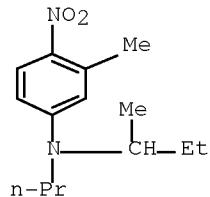
RN 821777-11-1 ZCPLUS

CN Benzenamine, N-butyl-N-ethyl-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-12-2 ZCPLUS

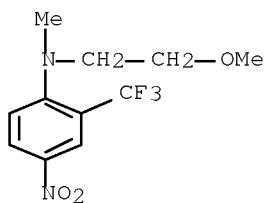
CN Benzenamine, 3-methyl-N-(1-methylpropyl)-4-nitro-N-propyl- (CA INDEX NAME)



RN 821777-13-3 ZCPLUS

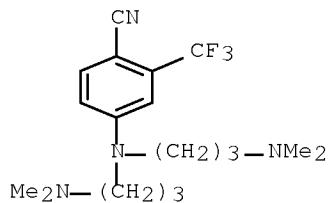
CN Benzenamine, N-(2-methoxyethyl)-N-methyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)

10/560012



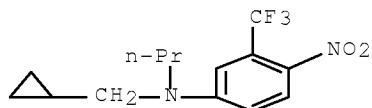
RN 821777-15-5 ZCPLUS

CN Benzonitrile, 4-[bis[3-(dimethylamino)propyl]amino]-2-(trifluoromethyl)-  
(CA INDEX NAME)



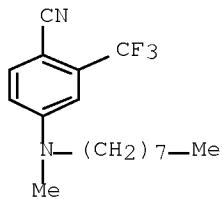
RN 821777-16-6 ZCPLUS

CN Benzenamine, N-(cyclopropylmethyl)-4-nitro-N-propyl-3-(trifluoromethyl)-  
(CA INDEX NAME)



RN 821777-17-7 ZCPLUS

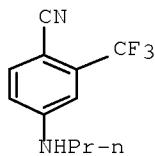
CN Benzonitrile, 4-(methyloctylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



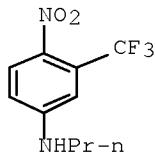
RN 821777-18-8 ZCPLUS

CN Benzonitrile, 4-(propylamino)-2-(trifluoromethyl)- (CA INDEX NAME)

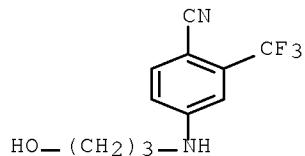
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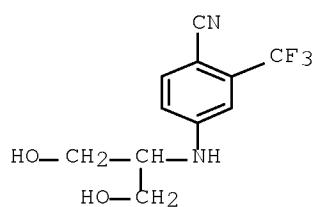
RN 821777-19-9 ZCPLUS  
CN Benzenamine, 4-nitro-N-propyl-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-20-2 ZCPLUS  
CN Benzonitrile, 4-[ (3-hydroxypropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

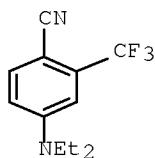


RN 821777-21-3 ZCPLUS  
CN Benzonitrile, 4-[ [2-hydroxy-1-(hydroxymethyl)ethyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

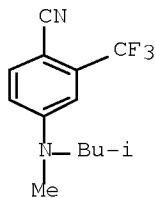


RN 821777-22-4 ZCPLUS  
CN Benzonitrile, 4-(diethylamino)-2-(trifluoromethyl)- (CA INDEX NAME)

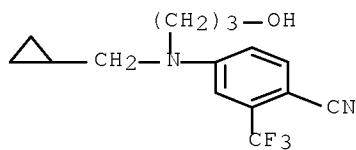
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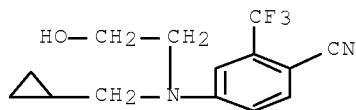
RN 821777-23-5 ZCPLUS  
CN Benzonitrile, 4-[methyl(2-methylpropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-25-7 ZCPLUS  
CN Benzonitrile, 4-[(cyclopropylmethyl)(3-hydroxypropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

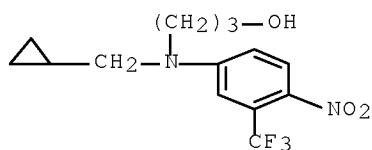


RN 821777-26-8 ZCPLUS  
CN Benzonitrile, 4-[(cyclopropylmethyl)(2-hydroxyethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



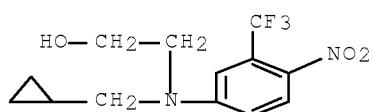
RN 821777-28-0 ZCPLUS  
CN 1-Propanol, 3-[(cyclopropylmethyl)[4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

10/560012



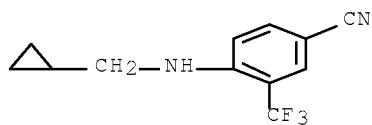
RN 821777-29-1 ZCPLUS

CN Ethanol, 2-[ (cyclopropylmethyl) [4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



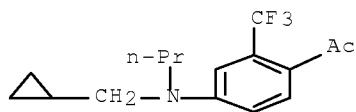
RN 821777-30-4 ZCPLUS

CN Benzonitrile, 4-[ (cyclopropylmethyl)amino]-3-(trifluoromethyl)- (CA INDEX NAME)



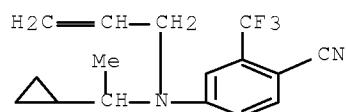
RN 821777-31-5 ZCPLUS

CN Ethanone, 1-[4-[ (cyclopropylmethyl)propylamino]-2-(trifluoromethyl)phenyl]- (CA INDEX NAME)

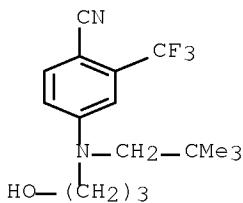


RN 821777-33-7 ZCPLUS

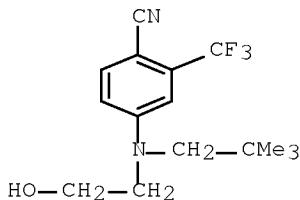
CN Benzonitrile, 4-[ (1-cyclopropylethyl)-2-propen-1-ylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



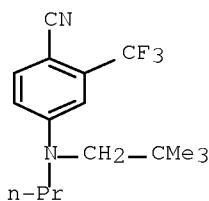
RN 821777-35-9 ZCPLUS  
CN Benzonitrile, 4-[(2,2-dimethylpropyl)(3-hydroxypropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-39-3 ZCPLUS  
CN Benzonitrile, 4-[(2,2-dimethylpropyl)(2-hydroxyethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

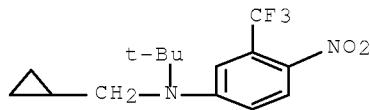


RN 821777-40-6 ZCPLUS  
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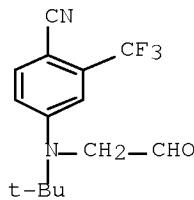
RN 821777-43-9 ZCPLUS  
CN Benzenamine, N-(cyclopropylmethyl)-N-(1,1-dimethylethyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)

10/560012



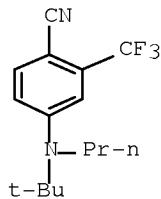
RN 821777-45-1 ZCPLUS

CN Benzonitrile, 4-[(1,1-dimethylethyl)(2-oxoethyl)amino]-2-(trifluoromethyl)-  
(CA INDEX NAME)



RN 821777-46-2 ZCAPLUS

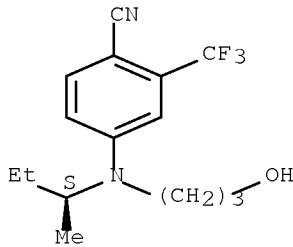
CN Benzonitrile, 4-[(1,1-dimethylethyl)propylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-47-3 ZCAPLUS

CN Benzonitrile, 4-[(3-hydroxypropyl)[(1S)-1-methylpropyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

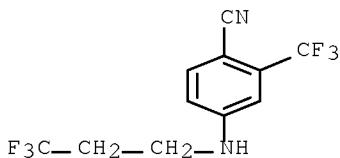
## Absolute stereochemistry.



10/560012

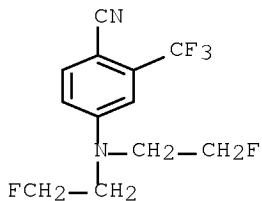
RN 821777-48-4 ZCPLUS

CN Benzonitrile, 2-(trifluoromethyl)-4-[ (3,3,3-trifluoropropyl)amino]- (CA INDEX NAME)



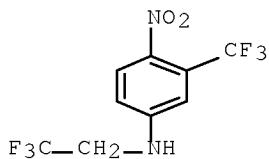
RN 821777-49-5 ZCPLUS

CN Benzonitrile, 4-[bis(2-fluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



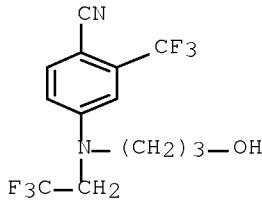
RN 821777-51-9 ZCPLUS

CN Benzenamine, 4-nitro-N-(2,2,2-trifluoroethyl)-3-(trifluoromethyl)- (CA INDEX NAME)



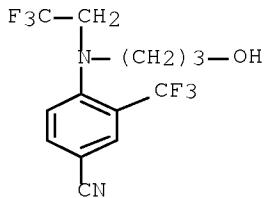
RN 821777-52-0 ZCPLUS

CN Benzonitrile, 4-[ (3-hydroxypropyl) (2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

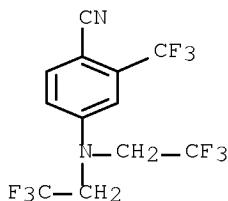


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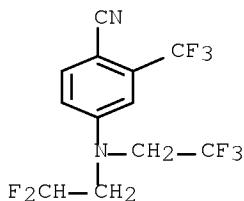
RN 821777-53-1 ZCPLUS  
CN Benzonitrile, 4-[ (3-hydroxypropyl) (2,2,2-trifluoroethyl)amino]-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-55-3 ZCPLUS  
CN Benzonitrile, 4-[bis(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

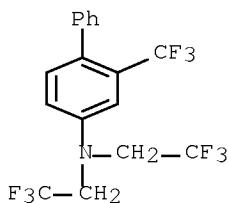


RN 821777-56-4 ZCPLUS  
CN Benzonitrile, 4-[ (2,2-difluoroethyl) (2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



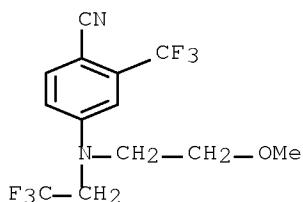
RN 821777-57-5 ZCPLUS  
CN [1,1'-Biphenyl]-4-amine, N,N-bis(2,2,2-trifluoroethyl)-2-(trifluoromethyl)- (CA INDEX NAME)

10/560012



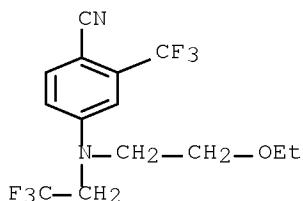
RN 821777-59-7 ZCPLUS

CN Benzonitrile, 4-[(2-methoxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



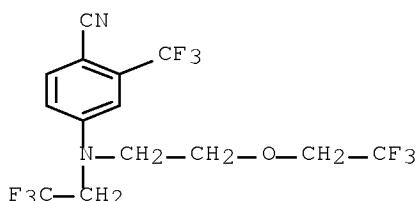
RN 821777-60-0 ZCPLUS

CN Benzonitrile, 4-[(2-ethoxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



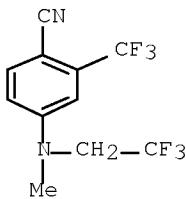
RN 821777-61-1 ZCPLUS

CN Benzonitrile, 4-[(2-(2,2,2-trifluoroethoxy)ethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

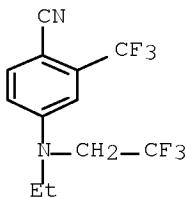


10/560012

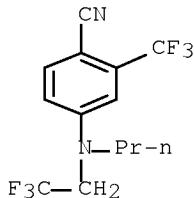
RN 821777-62-2 ZCPLUS  
CN Benzonitrile, 4-[methyl(2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-  
(CA INDEX NAME)



RN 821777-63-3 ZCPLUS  
CN Benzonitrile, 4-[ethyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-  
(CA INDEX NAME)

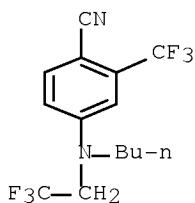


RN 821777-64-4 ZCPLUS  
CN Benzonitrile, 4-[propyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-  
(CA INDEX NAME)

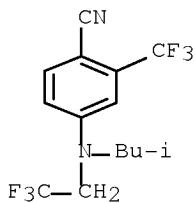


RN 821777-65-5 ZCPLUS  
CN Benzonitrile, 4-[butyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-  
(CA INDEX NAME)

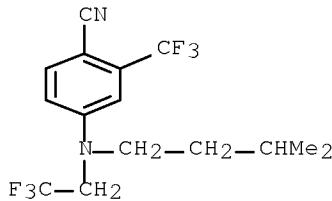
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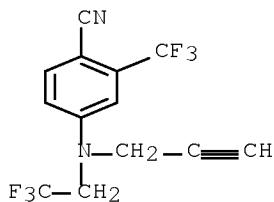
RN 821777-67-7 ZCPLUS  
CN Benzonitrile, 4-[(2-methylpropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-69-9 ZCPLUS  
CN Benzonitrile, 4-[(3-methylbutyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

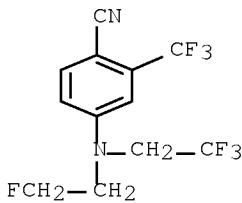


RN 821777-70-2 ZCPLUS  
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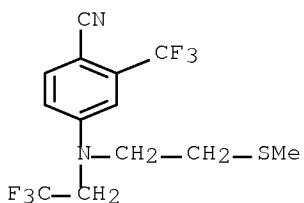


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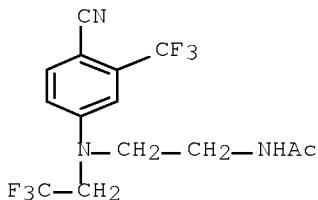
RN 821777-71-3 ZCPLUS  
CN Benzonitrile, 4-[(2-fluoroethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-72-4 ZCPLUS  
CN Benzonitrile, 4-[(2-(methylthio)ethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

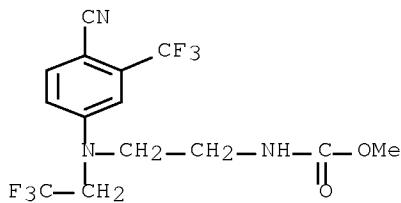


RN 821777-74-6 ZCPLUS  
CN Acetamide, N-[2-[(4-cyano-3-(trifluoromethyl)phenyl)(2,2,2-trifluoroethyl)amino]ethyl]- (CA INDEX NAME)



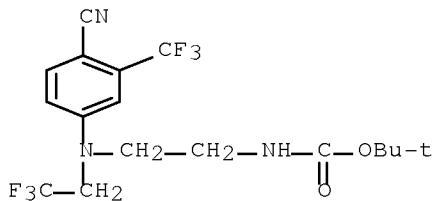
RN 821777-75-7 ZCPLUS  
CN Carbamic acid, [2-[(4-cyano-3-(trifluoromethyl)phenyl)(2,2,2-trifluoroethyl)amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

10/560012



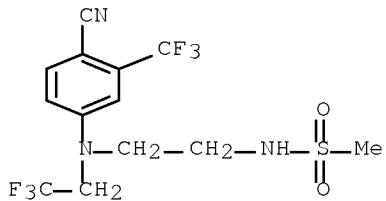
RN 821777-76-8 ZCPLUS

CN Carbamic acid, [2-[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



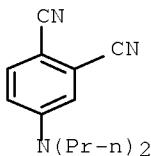
RN 821777-77-9 ZCPLUS

CN Methanesulfonamide, N-[2-[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl- (CA INDEX NAME)



RN 821777-78-0 ZCPLUS

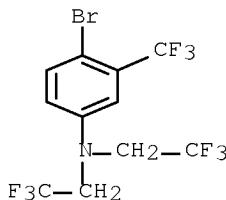
CN 1,2-Benzeneddicarbonitrile, 4-(dipropylamino)- (CA INDEX NAME)



RN 821778-33-0 ZCPLUS

10/560012

CN Benzenamine, 4-bromo-N,N-bis(2,2,2-trifluoroethyl)-3-(trifluoromethyl)-  
(CA INDEX NAME)

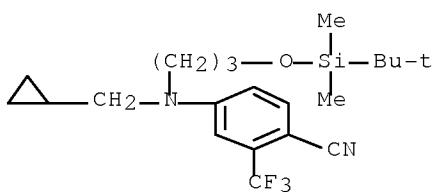


IT 821777-79-1P 821777-80-4P 821777-85-9P  
821777-86-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of substituted anilines as androgen receptor modulators)

RN 821777-79-1 ZCPLUS

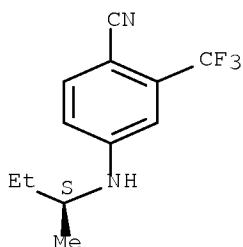
CN Benzonitrile, 4-[(cyclopropylmethyl)[3-[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-80-4 ZCPLUS

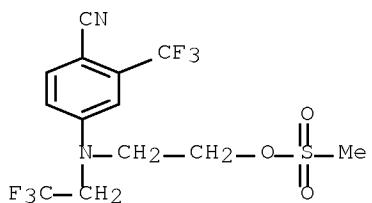
CN Benzonitrile, 4-[(1S)-1-methylpropyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

Absolute stereochemistry.



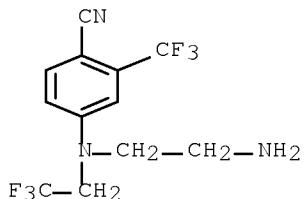
RN 821777-85-9 ZCPLUS

CN Benzonitrile, 4-[(2-[(methylsulfonyl)oxy]ethyl)(2,2,2-trifluoroethyl)]amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-86-0 ZCPLUS

CN Benzonitrile, 4-[(2-aminoethyl)(2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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DICTIONARY FILE UPDATES: 11 MAR 2009 HIGHEST RN 1119363-64-2

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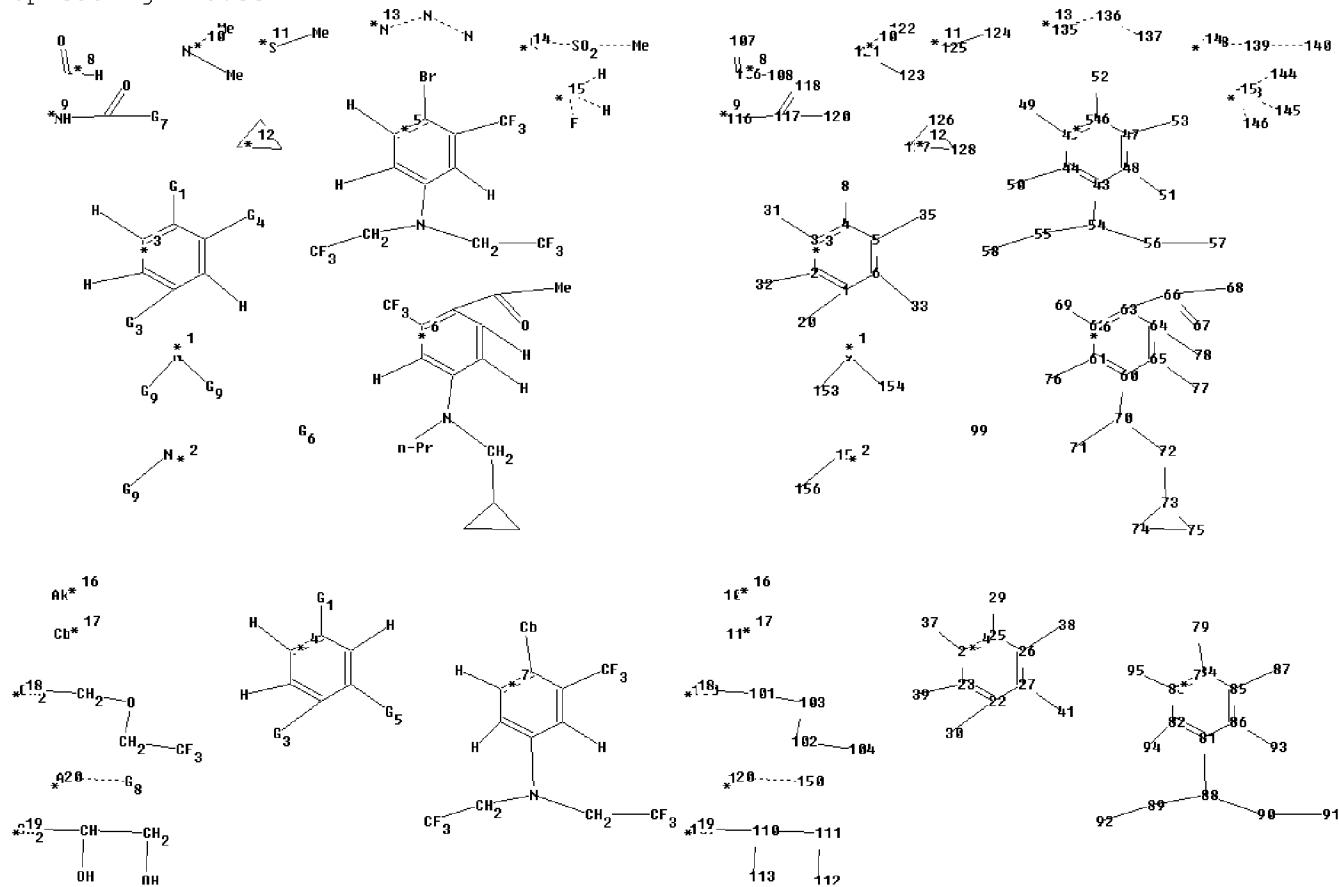
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<http://www.cas.org/support/stngen/stndoc/properties.html>

Uploading L26.str



10/560012

chain nodes :

8 9 10 11 15 20 29 30 31 32 33 35 37 38 39 41 49 50 51 52 53  
54 55 56 57 58 66 67 68 69 70 71 72 76 77 78 79 87 88 89 90 91  
92 93 94 95  
99 100 101 102 103 104 106 107 108 109 110 111 112 113 115 116 117  
118 120 121  
122 123 124 125 135 136 137 138 139 140 143 144 145 146 150 153 154  
156

ring nodes :

1 2 3 4 5 6 22 23 24 25 26 27 43 44 45 46 47 48 60 61 62 63  
64 65 73 74 75 81 82 83 84 85 86 126 127 128

chain bonds :

1-20 2-32 3-31 4-8 5-35 6-33 9-153 9-154 15-156 22-30 23-39 24-37 25-29  
26-38 27-41 43-54 44-50 45-49 46-52 47-53 48-51 54-55 54-56 55-58 56-57  
60-70 61-76  
62-69 63-66 64-78 65-77 66-67 66-68 70-71 70-72 72-73 79-84 81-88 82-94  
83-95 85-87  
86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-108  
106-107 109-110  
110-111 110-113 111-112 115-150 116-117 117-118 117-120 121-122 121-123  
124-125 135-136  
136-137 138-139 139-140 143-144 143-145 143-146

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-  
48  
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 73-74 73-75  
74-75 81-82  
81-86 82-83 83-84 84-85 85-86 126-127 126-128 127-128

exact/norm bonds :

1-20 4-8 5-35 9-153 9-154 15-156 22-30 25-29 27-41 43-54 60-70 66-67  
73-74 73-75 74-75 81-88 106-107 110-113 115-150 116-117 117-118 117-120  
126-127 126-128  
127-128 135-136 136-137 138-139 139-140 143-144 143-145 143-146

exact bonds :

2-32 3-31 6-33 23-39 24-37 26-38 44-50 45-49 46-52 47-53 48-51 54-55  
54-56 55-58 56-57 61-76 62-69 63-66 64-78 65-77 66-68 70-71 70-72 72-73  
79-84 82-94 83-95  
85-87 86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-  
108 109-110  
110-111 111-112 121-122 121-123 124-125

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-  
48  
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 81-82 81-86  
82-83 83-84  
84-85 85-86

isolated ring systems :

containing 1 : 22 : 43 : 60 : 81 :

G1:CN,NO2

G3:[\*1], [\*2]

G4:CF3,C1,NO2,CH3,OH,CN

G5:CH3,CF3,NO2,C1

G6:[\*3], [\*4], [\*5], [\*6], [\*7]

10/560012

G7:CH3,MeO,t-BuO

G8:CF3,OH,MeO,EtO,NH2,[\*8],[\*9],[\*10],[\*11],[\*12],[\*13],[\*14],[\*15]

G9:[\*16],[\*17],[\*18],[\*19],[\*20]

Hydrogen count :

9:= exact 0 15:= exact 1

Connectivity :

9:3 E exact RC ring/chain 10:1 E exact RC ring/chain 11:1 E exact RC ring/chain  
15:2 E exact RC ring/chain 79:1 E exact RC ring/chain 115:2 E exact RC ring/chain  
125:2 E exact  
RC ring/chain 126:2 E exact RC ring/chain 128:2 E exact RC ring/chain 138:2 E  
exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom  
15:CLASS 20:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 29:CLASS  
30:CLASS 31:CLASS  
32:CLASS 33:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 41:CLASS 43:Atom  
44:Atom 45:Atom  
46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS  
54:CLASS 55:CLASS  
56:CLASS 57:CLASS 58:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom  
66:CLASS  
67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:Atom 74:Atom  
75:Atom 76:CLASS 77:CLASS  
78:CLASS 79:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:CLASS  
88:CLASS  
89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 95:CLASS 99:CLASS  
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102:CLASS 103:CLASS 104:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS  
110:CLASS 111:CLASS  
112:CLASS 113:CLASS 115:CLASS 116:CLASS 117:CLASS 118:CLASS 120:CLASS  
121:CLASS 122:CLASS  
123:CLASS 124:CLASS 125:CLASS 126:Atom 127:Atom 128:Atom 135:CLASS 136:CLASS  
137:CLASS  
138:CLASS 139:CLASS 140:CLASS 143:CLASS 144:CLASS 145:CLASS 146:CLASS  
150:CLASS 153:CLASS  
154:CLASS 156:CLASS

Generic attributes :

11:

Saturation : Saturated

79:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

Node 10: Limited

C,C7

Node 11: Limited

C,C6

Node 79: Limited

C,C6

Node 115: Limited

C,C6

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=> d stat que L70
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L26      STR
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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

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L32      SCR 1840 OR 2043 OR 1951
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L47      135 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L38 AND L3
L48      16 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L3 NOT L47
L50      1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L48 AND BR/ELS AND
          9/F
L51      10 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L48 NOT BR/ELS
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L53      7 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L50 OR L52
L54      142 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L47 OR L53
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L57	68	SEA FILE=ZCPLUS SPE=ON ABB=ON PLU=ON L56
L58	49	SEA FILE=ZCPLUS SPE=ON ABB=ON PLU=ON L57 AND P/DT
L59	19	SEA FILE=ZCPLUS SPE=ON ABB=ON PLU=ON L57 NOT L58
L60	16	SEA FILE=ZCPLUS SPE=ON ABB=ON PLU=ON L59 AND PY<2004
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L63	30	SEA FILE=ZCPLUS SPE=ON ABB=ON PLU=ON L58 AND AD<20030610
L64	51	SEA FILE=ZCPLUS SPE=ON ABB=ON PLU=ON (L60 OR L61 OR L62 OR L63)
L66	142	SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L55 AND L54
L67	366	SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L56 OR L66
L68	68	SEA FILE=ZCPLUS SPE=ON ABB=ON PLU=ON L67
L70	51	SEA FILE=ZCPLUS SPE=ON ABB=ON PLU=ON L68 AND L64

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=> file zcaplus
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10/560012

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FILE COVERS 1907 - 12 Mar 2009 VOL 150 ISS 11  
FILE LAST UPDATED: 11 Mar 2009 (20090311/ED)

ZCPlus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCPLUS' FILE

=> d ibib abs hitstr L70 1-51

L70 ANSWER 1 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2006:1342415 ZCPLUS Full-text  
DOCUMENT NUMBER: 146:89971  
TITLE: Nile red luminescent compound emitting red light,  
process for producing the same and luminescence  
element utilizing the same  
INVENTOR(S): Nakaya, Tadao; Tajima, Akio; Saikawa, Tomoyuki;  
Takano, Shinji; Yamauchi, Takao; Mori, Hidemasa  
PATENT ASSIGNEE(S): Hirose Engineering Co., Ltd, Japan  
SOURCE: U.S. Pat. Appl. Publ., 55pp., Division of U.S. Ser.  
No. 501,398.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060287524	A1	20061221	US 2006-486111	20060831
US 20050113575	A1	20050526	US 2004-501398	20040715 <--
PRIORITY APPLN. INFO.:			US 2004-501398	A3 20040715
			JP 2002-12222	A 20020121 <--
			JP 2002-12224	A 20020121 <--
			JP 2002-14881	A 20020123 <--
			JP 2002-172127	A 20020612 <--
			WO 2003-JP477	W 20030121 <--

OTHER SOURCE(S): MARPAT 146:89971

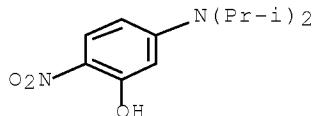
AB Luminescent derivs. of 9-amino-5H-benzo[a]phenoxazin-5-one (Nile Red derivs.) and methods for producing them are described. Electroluminescent devices employing the compds. are also described. The patent also describes the preparation of unclaimed luminescent derivs. of 9-amino-5H-benzo[a]phenothiazin-5-one.

IT 398482-49-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(luminescent aminobenzophenoxazinone derivs. and their preparation and light-emitting devices using them)

RN 398482-49-0 ZCPLUS

CN Phenol, 5-[bis(1-methylethyl)amino]-2-nitro- (CA INDEX NAME)



L70 ANSWER 2 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2005:902613 ZCPLUS Full-text  
 DOCUMENT NUMBER: 143:248160  
 TITLE: Preparation of benzamides for promoting apoptosis  
 INVENTOR(S): Bajji, Ashok C.; Arranz, Esther; Srinivasan, Jayasree M.; Delmar, Eric; Slade, Rachel; Willardsen, Jon Adam  
 PATENT ASSIGNEE(S): Myriad Genetics, Incorporated, USA  
 SOURCE: U.S. Pat. Appl. Publ., 121 pp., Cont.-in-part of Appl. No. PCT/US03/22183.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050187300	A1	20050825	US 2005-39275	20050118 <--
WO 2004006858	A2	20040122	WO 2003-US22183	20030715 <--
WO 2004006858	A3	20040429		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			US 2002-396266P	P 20020715 <--
			US 2002-396773P	P 20020716 <--
			WO 2003-US22183	A2 20030715

OTHER SOURCE(S): CASREACT 143:248160; MARPAT 143:248160

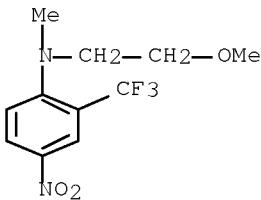
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Benzamides, e.g. I (R<sub>2</sub>, R<sub>3</sub> = halo, C<sub>1</sub>-C<sub>6</sub>-haloalkyl; R<sub>4</sub>, R<sub>5</sub> = C<sub>1</sub>-C<sub>6</sub>-alkyl; R<sub>6</sub> = H, halo; R<sub>7</sub> = halo, C<sub>1</sub>-C<sub>4</sub>-haloalkyl) and II [R<sub>11</sub>, R<sub>12</sub>, R<sub>13</sub>, R<sub>14</sub>, R<sub>15</sub>, R<sub>16</sub>, R<sub>17</sub>, R<sub>18</sub> = H, halo, N<sub>3</sub>, OH, SH, cyano, C<sub>1</sub>-C<sub>6</sub>-(halo)(hydroxy)alkyl, C<sub>2</sub>-C<sub>6</sub>-alkenyl, C<sub>2</sub>-C<sub>6</sub>-alkenyloxy, C<sub>2</sub>-C<sub>6</sub>-alkynyl, C<sub>1</sub>-C<sub>6</sub>-alkylsulfonamide, carbocycle, heterocyclyl, (hetero)aryl, NR<sub>50</sub>R<sub>51</sub>, NR<sub>50</sub>COR<sub>40</sub>, CONR<sub>50</sub>R<sub>51</sub>, C(:G<sub>1</sub>)G<sub>2</sub>R<sub>41</sub>, etc.; R<sub>40</sub> = H, OH, C<sub>1</sub>-C<sub>6</sub>-alkyl, C<sub>2</sub>-C<sub>6</sub>-alkenyl, C<sub>2</sub>-C<sub>6</sub>-alkynyl, C<sub>1</sub>-C<sub>6</sub>-alkoxy, C<sub>2</sub>-C<sub>6</sub>-alkenyloxy, C<sub>2</sub>-C<sub>6</sub>-alkynyl, C<sub>1</sub>-C<sub>6</sub>-alkylthiol; R<sub>41</sub> = H, C<sub>1</sub>-C<sub>6</sub>-alkyl, C<sub>2</sub>-C<sub>6</sub>-alkenyl, C<sub>2</sub>-C<sub>6</sub>-alkynyl; R<sub>50</sub>, R<sub>51</sub> = H, OH, C<sub>1</sub>-C<sub>10</sub>-(halo)alkyl, C<sub>2</sub>-C<sub>10</sub>-alkenyl, C<sub>2</sub>-C<sub>10</sub>-alkynyl, C<sub>1</sub>-C<sub>10</sub>-alkoxy, C<sub>1</sub>-C<sub>10</sub>-alkylthiol, C<sub>2</sub>-C<sub>10</sub>-alkenyloxy, C<sub>2</sub>-C<sub>10</sub>-alkynyl, C<sub>2</sub>-C<sub>6</sub>-hydroxyalkyl, etc.; R<sub>19</sub> = H, C<sub>1</sub>-C<sub>6</sub>-alkyl;

R20 = haloalkyl, C2-C6-alkoxy, C2-C6-alkyl, alkylene-O-R8, alkylene-R8, alkylene(R8R9), alkylene = C1-C6-alkylene, R8, R9 = cycloalkyl, aryl, heterocyclyl, heteroaryl; Z = O, NR21, S, R21 = H, C1-C6-alkyl], were prepared to promote apoptosis. To illustrate the synthesis, reacting 3-O2NC6H4OH with PhCH2CH2OH gave 3-O2NC6H4OCH2CH2Ph which was reduced to the amine and acylated with 5-chlorosalicylic acid to give benzamide III.

IT 821777-13-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of benzamide derivs. for promoting apoptosis)  
 RN 821777-13-3 ZCPLUS  
 CN Benzenamine, N-(2-methoxyethyl)-N-methyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



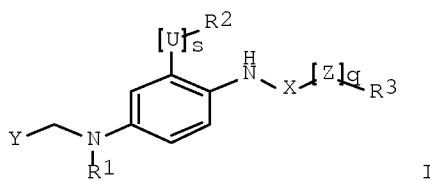
L70 ANSWER 3 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2004:802711 ZCPLUS Full-text  
 DOCUMENT NUMBER: 141:314020  
 TITLE: Preparation of substituted p-diaminobenzene derivatives as openers of the KCNQ family potassium ion channels  
 INVENTOR(S): Khanzhin, Nikolay; Rottlaender, Mario; Ritzen, Andreas; Watson, William Patrick  
 H. Lundbeck A/S, Den.  
 PATENT ASSIGNEE(S):  
 SOURCE: PCT Int. Appl., 176 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004082677	A1	20040930	WO 2004-DK186	20040318 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004222626	A1	20040930	AU 2004-222626	20040318 <--
CA 2519582	A1	20040930	CA 2004-2519582	20040318 <--

EP 1613303	A1	20060111	EP 2004-721472	20040318 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
BR 2004008437	A	20060404	BR 2004-8437	20040318 <--
CN 1761464	A	20060419	CN 2004-80007507	20040318 <--
JP 2006520759	T	20060914	JP 2006-504330	20040318 <--
IN 2005CN02347	A	20070831	IN 2005-CN2347	20050921 <--
NO 2005004848	A	20051020	NO 2005-4848	20051020 <--
US 20060183791	A1	20060817	US 2005-550448	20051116 <--
PRIORITY APPLN. INFO.:			DK 2003-441	A 20030321 <--
			US 2003-456698P	P 20030321 <--
			WO 2004-DK186	W 20040318

OTHER SOURCE(S): CASREACT 141:314020; MARPAT 141:314020

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AB The title anilines I [s = 0-1; U = O, S, SO<sub>2</sub>, etc.; q = 0-1; X = CO, SO<sub>2</sub>; with the proviso that q = 0 when X = SO<sub>2</sub>; Z = O, S; R1 = H, alk(en/yn)yl, cycloalk(en)yl, etc.; R2 = H, alk(en/yn)yl, cycloalk(en)yl, etc.; R3 = alk(en/yn)yl, cycloalk(en)yl, heterocycloalk(en)yl, etc.; Y = (un)substituted Ph, naphthyl, thieryl, etc.], useful for the prevention, treatment or inhibition of a disorder being responsive to an increased ion flow in a potassium channel, were prepared and formulated. Thus, reductive amination of Pr (4-amino-2-methylphenyl)carbamate (preparation given) with benzofuran-2-carbaldehyde in the presence of NaBH<sub>3</sub>CN afforded 43% Pr {4-[ (benzofuran-2-ylmethyl)amino]-2-methylphenyl}carbamate. The compds. I have an EC<sub>50</sub> of <2000nM, in most cases <200nM and in many cases <200nM in KCNQ2 channel assay.

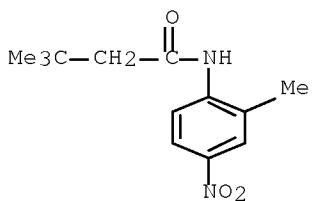
IT 335204-56-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted p-diaminobenzene derivs. as openers of the KCNQ family potassium ion channels)

RN 335204-56-3 ZCAPLUS

CN Butanamide, 3,3-dimethyl-N-(2-methyl-4-nitrophenyl)- (CA INDEX NAME)



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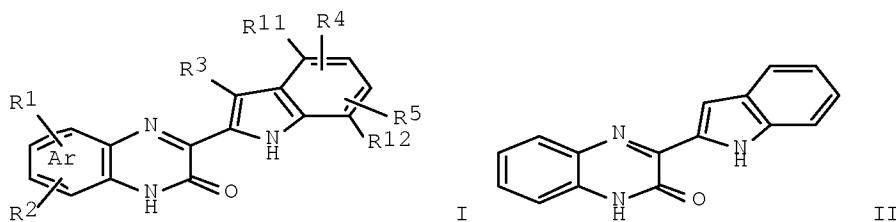
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 4 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2004:430796 ZCPLUS Full-text  
DOCUMENT NUMBER: 141:7139  
TITLE: Preparation of indolylquinoxalinones for treating hyperproliferative disorders and diseases associated with angiogenesis  
INVENTOR(S): Ladouceur, Gaetan H.; Bear, Brian; Bi, Cheng; Brittelli, David R.; Burke, Michael J.; Chen, Gang; Cook, James; Dumas, Jacques; Sibley, Robert; Turner, Michael R.  
PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA  
SOURCE: PCT Int. Appl., 217 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004043950	A1	20040527	WO 2003-US36003	20031110 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2505819	A1	20040527	CA 2003-2505819	20031110 <--
AU 2003290744	A1	20040603	AU 2003-290744	20031110 <--
EP 1565455	A1	20050824	EP 2003-783328	20031110 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003016169	A	20050927	BR 2003-16169	20031110 <--
CN 1738814	A	20060222	CN 2003-80108639	20031110 <--
JP 2006509840	T	20060323	JP 2005-507146	20031110 <--
MX 2005004779	A	20050722	MX 2005-4779	20050504 <--
US 20060004011	A1	20060105	US 2005-534215	20050506
NO 2005002796	A	20050609	NO 2005-2796	20050609 <--
PRIORITY APPLN. INFO.:			US 2002-425490P	P 20021112 <--
			US 2003-460915P	P 20030407 <--
			US 2003-484202P	P 20030630
			WO 2003-US36003	W 20031110

OTHER SOURCE(S): MARPAT 141:7139

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**AB** The invention relates to title compds. I [wherein Ar = 6-membered aromatic ring containing 0-2 N atoms; R1 and R2 = independently H, halo, CF<sub>3</sub>, acyl, piperidinyl, piperazinyl, morpholinyl, or (un)substituted alkyl, alkoxy, amino, pyrrolidinyl, Ph, etc.; R3 = H, alkyl, OH, NO<sub>2</sub>, NH<sub>2</sub>, alkylamino, alkoxyamino, or (un)substituted benzoylamino; R4 = H, OH, halo, CN, acyl, sulfamoyl, trialkylsiloxy, tetrazolyl, thienyl, pyrrolyl, pyrimidinyl, oxazolyl, furanyl, or (un)substituted alkyl, alkenyl, alkynyl, alkoxy, amino, oxadiazolyl, Ph, pyridyl(oxy), carbamoyl; R11 and R12 = independently H, F, or Cl with the proviso that when one of R11 and R12 = F or Cl, the other must be H; and pharmaceutically acceptable salts and esters thereof]. The invention also relates to the use of I and their pharmaceutical compns. for treating hyperproliferative disorders and diseases associated with angiogenesis (no data). Examples include representative syntheses for compds. of the invention, pharmaceutical compns. comprising them, and tumor model assays (no specific data given). For instance, N-Boc-indole was coupled with di-Me oxalate using t-BuLi to give tert-Bu 2-[methoxy(oxo)acetyl]-1H-indole-1-carboxylate (72%). Cyclization of the dione with 1,2-phenylenediamine in AcOH afforded the quinoxalinone II (77%).

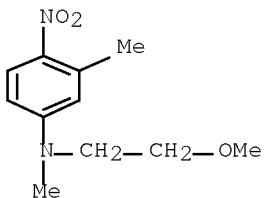
**IT** 694533-16-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of indolylquinoxalinones for treating hyperproliferative disorders and diseases associated with angiogenesis)

**RN** 694533-16-9 ZCPLUS

**CN** Benzenamine, N-(2-methoxyethyl)-N,3-dimethyl-4-nitro- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 5 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:287838 ZCPLUS Full-text

DOCUMENT NUMBER: 140:321373

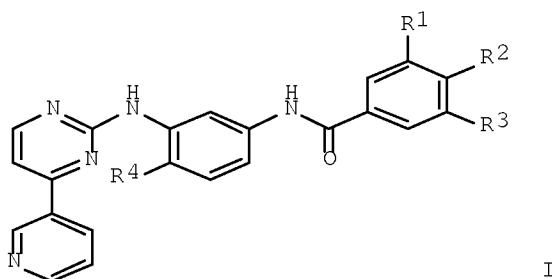
TITLE: Preparation of novel pyrimidine amides as protein kinase inhibitors

INVENTOR(S): Manley, Paul William; Breitenstein, Werner; Jacob,

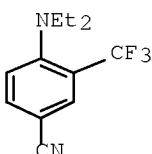
PATENT ASSIGNEE(S): Sandra; Furet, Pascal  
 Novartis Ag, Switz.; Novartis Pharma GmbH  
 SOURCE: PCT Int. Appl., 57 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029038	A1	20040408	WO 2003-EP10724	20030926 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SY, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2499822	A1	20040408	CA 2003-2499822	20030926 <--
AU 2003270277	A1	20040419	AU 2003-270277	20030926 <--
AU 2003270277	B2	20070823		
EP 1546127	A1	20050629	EP 2003-750639	20030926 <--
EP 1546127	B1	20070808		
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BR 2003014797	A	20050726	BR 2003-14797	20030926 <--
CN 1684951	A	20051019	CN 2003-823213	20030926 <--
CN 100404528	C	20080723		
JP 2006508064	T	20060309	JP 2004-539039	20030926 <--
AT 369355	T	20070815	AT 2003-750639	20030926 <--
ES 2288615	T3	20080116	ES 2003-750639	20030926 <--
NZ 538930	A	20080430	NZ 2003-538930	20030926 <--
ZA 2005002304	A	20060426	ZA 2005-2304	20050318 <--
MX 2005003253	A	20050608	MX 2005-3253	20050323 <--
IN 2005CN00464	A	20070406	IN 2005-CN464	20050323 <--
KR 876055	B1	20081226	KR 2005-705204	20050325 <--
NO 2005001966	A	20050422	NO 2005-1966	20050422 <--
HK 1080459	A1	20080215	HK 2005-111972	20051223 <--
US 20060142577	A1	20060629	US 2006-528913	20060105 <--
KR 2007098940	A	20071005	KR 2007-719251	20070823 <--
IN 2007CN04330	A	20080125	IN 2007-CN4330	20071001 <--
PRIORITY APPLN. INFO.:			GB 2002-22514	A 20020927 <--
			WO 2003-EP10724	W 20030926
			IN 2005-CN464	A3 20050323
			KR 2005-705204	A3 20050325

OTHER SOURCE(S): MARPAT 140:321373  
 GI



- AB The title substituted N-(3-benzoylaminophenyl)-4-pyridyl-2-pyrimidinamines [I; R1 = H and R2 = NR5R6, or R1 = NR5R6 and R2 = H; R3 = alkyl, fluoroalkyl, hydroxyalkyl, carbamoyl; R4 = H, alkyl, halo; R5 and R6 = H, alkyl, hydroxyalkyl, etc. or NR5R6 = (un)substituted (un)saturated 5-7 membered ring optionally containing heteroatoms], useful for the therapy of a disease which responds to an inhibition of protein kinase activity, especially a neoplastic disease (e.g., leukemia), were prepared and formulated. Thus, amidation of 4-methyl-N-[4-(3-pyridinyl)-2-pyrimidinyl]-1,3-benzenediamine with 4-diethylamino-3-(trifluoromethyl)benzoic acid (preparation given) afforded I [R1 = H; R2 = NET2; R3 = CF3; R4 = Me] which showed IC50 of 50-100 nM against c-Abl and IC50 of 200-500 nM against Bcr-Abl (in vitro inhibition data).
- IT 677704-53-9P, 4-(Diethylamino)-3-(trifluoromethyl)benzonitrile  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of novel N-[3-(pyrimidin-2-ylamino)phenyl] benzamides as protein kinase inhibitors)
- RN 677704-53-9 ZCAPLUS
- CN Benzonitrile, 4-(diethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 6 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:591159 ZCAPLUS Full-text  
 DOCUMENT NUMBER: 139:157136  
 TITLE: Nile red type compound emitting red light, process for producing the same, and luminescent element utilizing the same  
 INVENTOR(S): Nakaya, Tadao; Tajima, Akio; Saikawa, Tomoyuki; Takano, Shinji; Yamauchi, Takao; Mori, Hidemasa  
 PATENT ASSIGNEE(S): Taiho Industries, Co. Ltd., Japan  
 SOURCE: PCT Int. Appl., 112 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese

10/560012

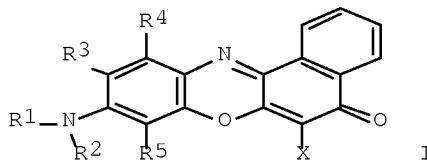
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003062213	A1	20030731	WO 2003-JP477	20030121 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2003277371	A	20031002	JP 2002-14881	20020123 <--
JP 2004018400	A	20040122	JP 2002-172127	20020612 <--
JP 2003277369	A	20031002	JP 2003-12498	20030121 <--
EP 1475372	A1	20041110	EP 2003-701142	20030121 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1620441	A	20050525	CN 2003-802508	20030121 <--
US 20050113575	A1	20050526	US 2004-501398	20040715 <--
PRIORITY APPLN. INFO.:				
		JP 2002-12222	A	20020121 <--
		JP 2002-12224	A	20020121 <--
		JP 2002-14881	A	20020123 <--
		JP 2002-172127	A	20020612 <--
		JP 2001-313245	A	20011010 <--
		WO 2003-JP477	W	20030121 <--

OTHER SOURCE(S): MARPAT 139:157136

GI



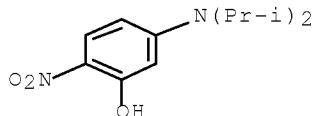
AB The invention relates to a Nile red-based red-emitting compound represented by I [R1-2 = H and alkyl; R3(R5) = H and may combine with R1(R2) to form a ring; R4 = H and may combine with R3 to form a ring; X = H, halo, and -CH(CN)Ar]. The compound is suited for use as a red-emitting material in an organic light emitting device.

IT 398482-49-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(nile red type compound for red-emitting organic LED)

RN 398482-49-0 ZCPLUS

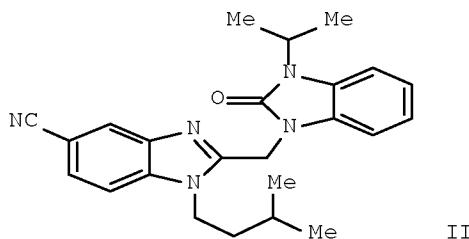
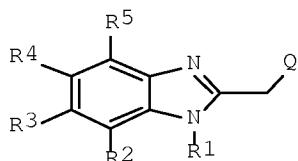
CN Phenol, 5-[bis(1-methylethyl)amino]-2-nitro- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 7 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:511082 ZCPLUS Full-text  
 DOCUMENT NUMBER: 139:85343  
 TITLE: Preparation of 2-(heterocyclmethyl)benzimidazoles as respiratory syncytial virus antiviral agents  
 INVENTOR(S): Yu, Kuo-long; Wang, Xiangdong; Sun, Yaxiong; Cianci, Christopher; Thuring, Jan Willem; Combrink, Keith; Meanwell, Nicholas; Zhang, Yi; Civiello, Rita L.  
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
 SOURCE: PCT Int. Appl., 149 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053344	A2	20030703	WO 2002-US39220	20021206 <--
WO 2003053344	A3	20031113		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20030207868	A1	20031106	US 2002-309505	20021204 <--
US 6919331	B2	20050719		
AU 2002362094	A1	20030709	AU 2002-362094	20021206 <--
EP 1461035	A2	20040929	EP 2002-797226	20021206 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
PRIORITY APPLN. INFO.:			US 2001-339025P	P 20011210 <--
			WO 2002-US39220	W 20021206 <--
OTHER SOURCE(S):	MARPAT	139:85343		
GI				



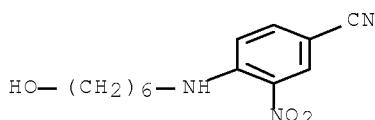
AB Title compds. I [wherein R1 = (CRaRb)nX; R2 = H; R3 = CONRhRi, CO2Rd, or (un)substituted alkyl; R4 = NH2, CONRhRi, heteroaryl, alkenyl, CO2Rd, N=CPh2, C(NOH)NH2, C(NH)NH2, or (un)substituted alkyl; R5 = CO2Rj or (un)substituted alkyl or alkenyl; Q = (un)substituted benzimidazolyl, benzotriazolyl, imidazopyridinyl, quinolinyl, quinazolinyl, benzyloxy, etc.; X = H or (un)substituted alkyl; Ra and Rb = independently H or (halo)alkyl; Rd = alkyl; Rh and Ri = independently H or alkyl; Rj = H or alkyl; n = 1-6; and pharmaceutically acceptable salts thereof] were prepared as antiviral compds. More particularly, the invention provides 2-(heterocyclymethyl)benzimidazole derivs. for the treatment of respiratory syncytial virus (RSV) infection. For example, 1-isopropyl-1,3-dihydrobenzimidazol-2-one was coupled with 2-chloromethyl-1-(3-methylbutyl)-1H-benzimidazole-5-carbonitrile in the presence of Cs2CO3 in DMF to give II (95%). Disclosed compds. protected HEp-2 cells from RSV-induced cytopathic effects with EC50 values between 50 µM and 0.001 µM, compared to an EC50 of 3 µM for ribavirin. I also displayed antiviral activity by reducing viral protein expression in HEp-2 cells with EC50 values between 50 µM and 0.001 µM, compared to an EC50 value of 3 µM for ribavirin. Thus, I and compns. comprising I are useful for the treatment of RSV infections.

IT 554457-74-8P 554458-11-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of (heterocyclymethyl)benzimidazoles as RSV antiviral agents)

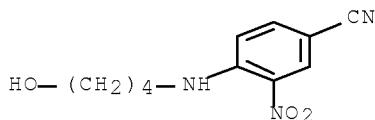
RN 554457-74-8 ZCAPLUS

CN Benzonitrile, 4-[(6-hydroxyhexyl)amino]-3-nitro- (CA INDEX NAME)



RN 554458-11-6 ZCAPLUS

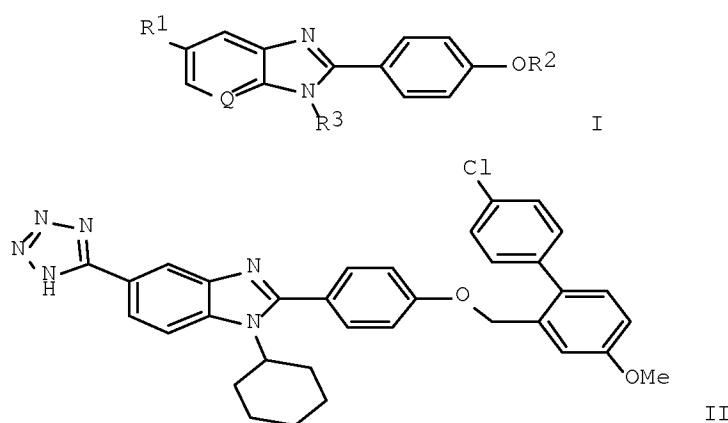
CN Benzonitrile, 4-[(4-hydroxybutyl)amino]-3-nitro- (CA INDEX NAME)



L70 ANSWER 8 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:261620 ZCPLUS Full-text  
 DOCUMENT NUMBER: 138:287673  
 TITLE: Preparation of phenylbenzimidazole compounds useful  
       for treating hepatitis C virus  
 INVENTOR(S): Priestley, Eldon Scott; Decicco, Carl P.; Hudyma,  
               Thomas W.; Zheng, Xiaofan  
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
 SOURCE: PCT Int. Appl., 74 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026587	A2	20030403	WO 2002-US30989	20020926 <--
WO 2003026587	A3	20031106		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002337765	A1	20030407	AU 2002-337765	20020926 <--
US 20030134853	A1	20030717	US 2002-259041	20020926 <--
EP 1429759	A2	20040623	EP 2002-773657	20020926 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 20040067976	A1	20040408	US 2003-648873	20030827 <--
US 6803374	B2	20041012		
PRIORITY APPLN. INFO.:			US 2001-324874P	P 20010926 <--
			US 2002-259041	B1 20020926 <--
			WO 2002-US30989	W 20020926 <--

OTHER SOURCE(S): MARPAT 138:287673  
 GI



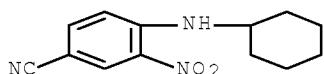
AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO<sub>2</sub>, PhCONHSO<sub>2</sub>, etc.; R2 = CH<sub>2</sub>-aryl, CHPh<sub>2</sub>, etc.; R3 = cycloalkyl] are prepared which are useful in treating viral hepatitis C. Thus, II was prepared and had an IC<sub>50</sub> of 0.14 μM against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 28096-55-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of phenylbenzimidazole compds. for treating hepatitis C viral infection)

RN 28096-55-1 ZCPLUS

CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)



L70 ANSWER 9 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2002:418358 ZCPLUS Full-text  
DOCUMENT NUMBER: 137:370024  
TITLE: Synthesis of some new 2-substituted-phenyl-1H-benzimidazole-5-carbonitriles and their potent activity against Candida species  
AUTHOR(S): Goker, Hakan; Kus, Canan; Boykin, David W.; Yildiz, Sulhiye; Altanlar, Nurten  
CORPORATE SOURCE: Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Ankara University, Ankara, 06100, Turk.  
SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(8), 2589-2596  
CODEN: BMECEP; ISSN: 0968-0896  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:370024  
AB New 2-substituted-phenyl-1H-benzimidazole-5-carboxylic acids, ethyl-5-carboxylate, -5-carboxamides, -5-carboxaldehyde, -5-chloro-, -5-

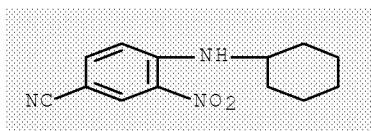
trifluoromethyl, and -5-carbonitriles, -6-carbonitrile were prepared and evaluated in vitro against Candida species. The cyano substituted compds. exhibited the greatest activity with MIC values of 3.12 µg/mL, values similar to that of fluconazole.

IT 28096-55-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and m.p. of 2-substituted-Ph-1H-benzimidazole-5-carbonitriles)

RN 28096-55-1 ZCPLUS

CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 10 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:122974 ZCPLUS Full-text

DOCUMENT NUMBER: 136:191436

TITLE: Nile-red luminescent compound, process for producing the same, and luminescent element utilizing the same

INVENTOR(S): Nakaya, Tadao; Yamauchi, Takao; Saikawa, Tomoyuki; Tajima, Akio; Mori, Hidemasa

PATENT ASSIGNEE(S): Taiho Industries, Co., Ltd, Japan

SOURCE: PCT Int. Appl., 67 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

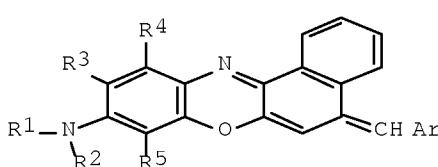
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012208	A1	20020214	WO 2001-JP5671	20010629 <--
W: CA, CN, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
US 20040054174	A1	20040318	US 2003-416586	20030513 <--
PRIORITY APPLN. INFO.:			JP 2000-236670	A 20000804 <--
			JP 2000-348516	A 20001115 <--
			WO 2001-JP5671	W 20010629 <--

OTHER SOURCE(S): MARPAT 136:191436

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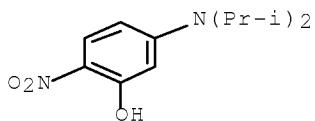
I

AB The invention provides a novel nile-red compound capable of emitting a nearly crimson red light; a novel process for producing the compound; and a luminescent compound which emits a nearly crimson red color at a high luminance. The nile-red luminescent compound is obtained by converting C=O in a nile-red compound into C=CH-Ar (wherein Ar is a fluorinated aromatic group) and incorporating an electron-donating group into the nile-red skeleton. The novel production process comprises reacting a nile-red dye with an electron-attracting aromatic MeCN. The nile-red based luminescent composition comprises a nile-red luminescent compound represented by I [R1 = R2 = C1-5 alkyl; R3 = H, or may be combined with R1 to form -CH2CH2-CR6R7- [R6 = R7 = H, and C1-5 alkyl, where the carbon in -CR6R7- is joined to the benzene ring]; R4 = H or may be combined with R3 to form naphthalene ring; R5 = H or may be combined with R2 to form -CH2CH2-CR8R9- [R8 = R9 = H and C1-5 alkyl, where the carbon in -CR8R9- is joined to the benzene ring]; Ar = fluorinated aroms.].

IT 398482-49-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (production of nile-red luminescent compound for electroluminescent device)

RN 398482-49-0 ZCPLUS

CN Phenol, 5-[bis(1-methylethyl)amino]-2-nitro- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 11 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2001:338479 ZCPLUS Full-text  
 DOCUMENT NUMBER: 134:353175  
 TITLE: Preparation of amides and ureas as activators of soluble guanylate cyclase  
 INVENTOR(S): Selwood, David; Glen, Robert; Reynolds, Karen; Wishart, Grant  
 PATENT ASSIGNEE(S): University College London, UK  
 SOURCE: PCT Int. Appl., 101 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

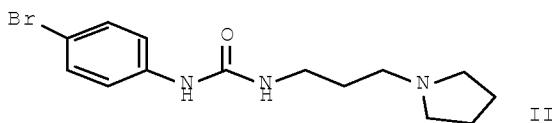
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032604	A1	20010510	WO 2000-GB4249	20001106 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				

10/560012

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
CA 2389773 A1 20010510 CA 2000-2389773 20001106 <--  
EP 1237849 A1 20020911 EP 2000-973061 20001106 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
JP 2003513064 T 20030408 JP 2001-534758 20001106 <--  
PRIORITY APPLN. INFO.: GB 1999-26286 A 19991105 <--  
US 2000-201382P P 20000502 <--  
WO 2000-GB4249 W 20001106 <--

OTHER SOURCE(S): MARPAT 134:353175

GI



AB The title compds. R4PZNR1R2 [I; R1, R2 = alkyl; R1R2 together form alkylene; Z = alkylene; P = a direct bond, X, Y, W, XY, YW, XYW (wherein W = O, S, NR3; R3 = H, alkyl; Y = UV; V = a direct bond, alkylene; U = CS, CO, SO2, C(:NR); R = H, OH, alkyl; X = O, NR6; R6 = H, alkyl, alkenyl, etc.); R4 = alkyl, alkenyl, alkynyl, etc.], useful in the activation of soluble guanylate cyclase, were prepared. E.g., synthesis of the urea II, starting with 4-bromoaniline and 1-(3-aminopropyl)pyrrolidine, was given. Biol. data for compds. I (e.g., IC50 for inhibition of platelet aggregation) were presented.

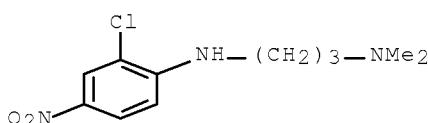
IT 338981-22-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amides and ureas as activators of soluble guanylate cyclase)

RN 338981-22-9 ZCPLUS

CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 12 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:63979 ZCPLUS Full-text

DOCUMENT NUMBER: 134:100871

TITLE: Benzimidazolone derivatives, method of preparation and their use as phosphodiesterase inhibitors

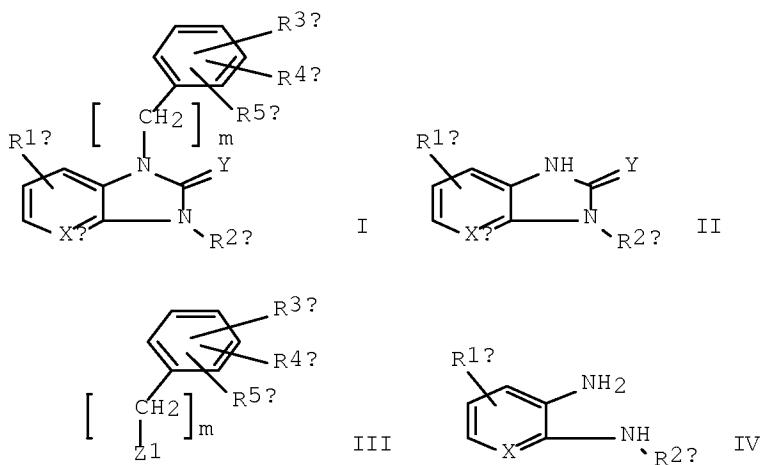
INVENTOR(S): Sawada, Kozo; Inoue, Takayuki; Sawada, Yuki; Mizutani,

Tsuyoshi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 159 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005770	A1	20010125	WO 2000-JP4687	20000712 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2379554	A1	20010125	CA 2000-2379554	20000712 <--
AU 2000058531	A	20010205	AU 2000-58531	20000712 <--
EP 1196391	A1	20020417	EP 2000-944421	20000712 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200200161	T2	20020521	TR 2002-161	20000712 <--
BR 2000013041	A	20020716	BR 2000-13041	20000712 <--
HU 2002002186	A2	20021228	HU 2002-2186	20000712 <--
HU 2002002186	A3	20030228		
JP 2003505376	T	20030212	JP 2001-511431	20000712 <--
ZA 2002000029	A	20030402	ZA 2002-29	20020102 <--
IN 2002KN00019	A	20050311	IN 2002-KN19	20020103 <--
MX 2002000340	A	20020621	MX 2002-340	20020109 <--
US 6582351	B1	20030624	US 2002-30979	20020116 <--
PRIORITY APPLN. INFO.:			AU 1999-1747	A 19990721 <--
			AU 1999-2730	A 19990909 <--
			WO 2000-JP4687	W 20000712 <--

OTHER SOURCE(S): MARPAT 134:100871  
 GI

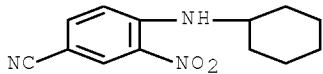


**AB** Benzimidazolone derivs. I, its prodrugs or pharmaceutically acceptable salts thereof, a method for their preparation, pharmaceutical compns. containing them, and usefulness in treatment or prevention of diseases mediated by cyclic guanosine-3',5'-monophosphate phosphodiesterase (cGMP-PDE) are claimed. In I, Xa = CH or N; ya = O, S; R1a = halogen, cyano, NO<sub>2</sub> carbamoyl, lower alkylcarbamoyl which may be substituted with a heterocyclic group, carboxy, protected carboxy, lower alkyl, halo(lower)alkyl, lower alkoxy, acyl, lower alkanesulfonyl. R2a = lower alkyl, cycloalkyl or heterocyclic group, among which the lower alkyl group may have 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, lower alkylamino, acylamino, lower alkoxy carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, carboxy, lower alkanesulfonyl, lower alkylenedioxy, carbamoyl, lower alkyl carbamoyl and sulfamoyl; and the cycloalkyl group and the heterocyclic group may have 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, lower alkanesulfonyl, lower alkyl, hydroxy(lower)alkyl, protected hydroxy(lower)alkyl, lower alkylenedioxy, carbamoyl and sulfamoyl. R3a, R4a and R5a = same or different, H, halogen, lower alkanoyl, carboxy, protected carboxy, carbamoyl, nitro, cyano, lower alkyl optionally substituted by hydroxy, lower alkoxy or lower-alkoxy-substituted aralkyl; or two of R3a, R4a and R5a may combine together to form a lower alkylenedioxy. M = 1, 2, provided that when R3a = H, R4a = lower alkoxy and R5a = H, halogen, cyano, lower alkyl, lower alkoxy, protected carboxy, carboxy or nitro, then (1) the lower alkyl for R2a has 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, carboxy, lower alkanesulfonyl, lower alkyl, hydroxy(lower)alkyl, protected hydroxy(lower)alkyl, lower alkylenedioxy, carbamoyl and sulfamoyl, (2) the cycloalkyl for R2a has 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, lower alkanesulfonyl, lower alkyl, hydroxy(lower)alkyl, protected hydroxy(lower)alkyl, lower alkylenedioxy, carbamoyl and sulfamoyl, (3) the heterocyclic group for R2a = pyrrolidinyl, dioxanyl and piperidyl which groups may be substituted with protected carboxy, acyl, lower alkanesulfonyl, carbamoyl or sulfamoyl, (4) R1a = carbamoyl, lower alkylcarbamoyl which may be substituted with a heterocyclic group, carboxy, protected carboxy, acyl, or lower alkanesulfonyl, (5) Xa = N; (6) m = 2; or

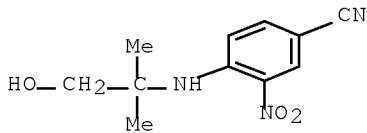
(7) yra = S. Pharmaceutical compns. containing the above compds. are claimed (with test data provided for 8 compds.) to be effective for treatment or prevention of diseases mediated by cGMP-PDE: angina, hypertension, pulmonary hypertension, congestive heart failure, glomerular diseases, renal tubulo-intestinal diseases, renal failure, atherosclerosis, conditions of reduced blood vessel patency, peripheral vascular disease, stroke, bronchitis, asthma, allergic rhinitis, urticaria, glaucoma, diseases characterized by disorders of gut motility, erectile dysfunction, female sexual dysfunction, impotence, diabetic complications, micturition disorder, or incontinence and storage of urine disorder. The method of preparation comprises reacting II with III (Z1 = halogen) in the presence of base. III are made by intramol. cyclization of IV (X = N). For example, to a solution of 1-(trans-4-hydroxycyclohexyl)-5-trifluoromethyl-2,3-dihydro-1H-benzimidazol-2-one (200 mg) in anhydrous DMF (2 mL) was added portionwise NaH (29.3 mg, 60% dispersion in mineral oil) at 5° under N<sub>2</sub> atmosphere, and the mixture was stirred at room temperature for 30 min. After adding 3,4-dimethoxybenzyl bromide (154 mg), the mixture was stirred at room temperature for 2 h. After workup, 3-(3,4-dimethoxybenzyl)-1-(trans-4-hydroxycyclohexyl)-5-trifluoromethyl-2,3-dihydro-1H-benzimidazol-2-one (217.9 mg) was obtained as a colorless solid.

IT 28096-55-1P, 4-Cyclohexylamino-3-nitrobenzonitrile  
 320405-95-6P, 4-(1,1-Dimethyl-2-hydroxyethylamino)-3-nitrobenzonitrile 320406-03-9P,  
 4-[(S)-1-Ethyl-2-hydroxyethyl]amino]-3-nitrobenzonitrile  
 320406-04-0P, 4-[(R)-1-Ethyl-2-hydroxyethyl]amino]-3-nitrobenzonitrile  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; benzimidazolone derivs., method of preparation and use as phosphodiesterase inhibitors)

RN 28096-55-1 ZCPLUS  
 CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)

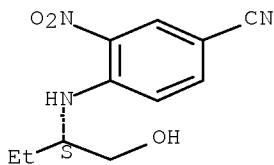


RN 320405-95-6 ZCPLUS  
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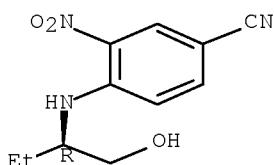
RN 320406-03-9 ZCPLUS  
 CN Benzonitrile, 4-[(1S)-1-(hydroxymethyl)propyl]amino]-3-nitro- (CA INDEX NAME)

Absolute stereochemistry.



RN 320406-04-0 ZCPLUS  
 CN Benzonitrile, 4-[(1R)-1-(hydroxymethyl)propyl]amino]-3-nitro- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 13 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2000:401817 ZCPLUS [Full-text](#)  
 DOCUMENT NUMBER: 133:30667  
 TITLE: Heteroaryl-containing thiourea derivatives useful as inhibitors of herpes viruses  
 INVENTOR(S): Bloom, Jonathan David; Digrandi, Martin Joseph;  
 Dushin, Russell George; Lang, Stanley Albert; O'Hara, Bryan Mark  
 PATENT ASSIGNEE(S): American Home Products Corporation, USA  
 SOURCE: PCT Int. Appl., 164 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 4  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034269	A1	20000615	WO 1999-US28892	19991206 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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US 6197803	B1	20010306	US 1999-447006	19991122 <--

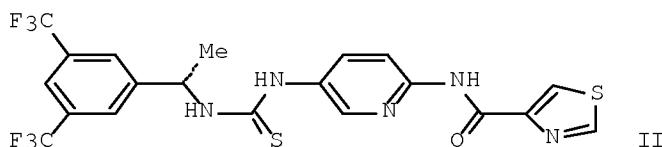
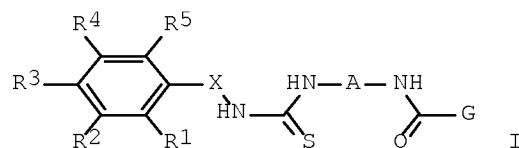
10/560012

US 6201013	B1	20010313	US 1999-444075	19991122 <--
CA 2351390	A1	20000615	CA 1999-2351390	19991206 <--
EP 1140913	A1	20011010	EP 1999-965143	19991206 <--
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BR 9916042	A	20011204	BR 1999-16042	19991206 <--
HU 2001004758	A2	20020429	HU 2001-4758	19991206 <--
HU 2001004758	A3	20020528		
JP 2002531558	T	20020924	JP 2000-586716	19991206 <--
AU 756043	B2	20030102	AU 2000-31122	19991206 <--
US 6262082	B1	20010717	US 2000-669483	20000925 <--
US 6271236	B1	20010807	US 2000-669943	20000926 <--
ZA 2001004373	A	20020918	ZA 2001-4373	20010528 <--
NO 2001002836	A	20010808	NO 2001-2836	20010608 <--
MX 2001005827	A	20010911	MX 2001-5827	20010608 <--
BG 105580	A	20020131	BG 2001-105580	20010608 <--
IN 2001KN00865	A	20050311	IN 2001-KN865	20010822 <--
IN 2001KN00866	A	20050311	IN 2001-KN866	20010822 <--
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US 6555561	B2	20030429		
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		US 1998-208540	A 19981209 <--	
		US 1998-150692P	P 19981209 <--	
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		US 1998-155192P	P 19981209 <--	
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		US 1998-208164	A 19981209 <--	
		US 1998-208559	A 19981209 <--	
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		US 1999-444782	A3 19991122 <--	
		WO 1999-US28892	W 19991206 <--	
		US 2000-669535	A3 20000926 <--	
		IN 2001-KN492	A3 20010508 <--	
		IN 2001-KN541	A3 20010522 <--	
		IN 2001-KN558	A3 20010525 <--	

OTHER SOURCE(S):

MARPAT 133:30667

GI



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO<sub>2</sub>, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, NR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>), or W-Y-(CH<sub>2</sub>)<sub>n</sub>-Z, provided that at least 1 of R1-R5 ≠ H; or R<sub>2</sub>R<sub>3</sub> or R<sub>3</sub>R<sub>4</sub> form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R<sub>6</sub>, R<sub>7</sub> = H, C1-6 alkyl or perhaloalkyl, or aryl; R<sub>8</sub> = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR<sub>7</sub>R<sub>8</sub> forms 3- to 7-membered heterocycloalkyl; A = heteroaryl; W = O, NR<sub>6</sub>, or bond; Y = CO, CO<sub>2</sub>, or bond; Z = C1-4 alkyl, CN, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, OCOR<sub>6</sub>, NR<sub>6</sub>COR<sub>7</sub>, OCONR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, SR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>) or Ph; G = aryl or heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH<sub>2</sub>; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 25 compds. in 2-4 bioassays. For instance, the pyridinylthiazolecarboxamide derivative II had an IC<sub>50</sub> of 0.001 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture.

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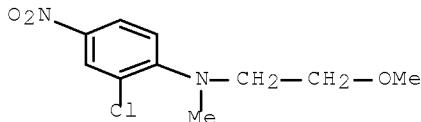
821777-03-1 1098071-56-7

RL: PRPH (Prophetic)

(Heteroaryl-containing thiourea derivatives useful as inhibitors of herpes viruses)

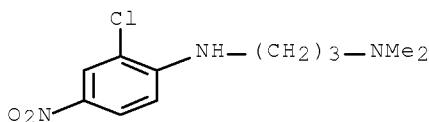
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CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



RN 338981-22-9 ZCPLUS

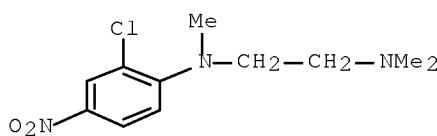
CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



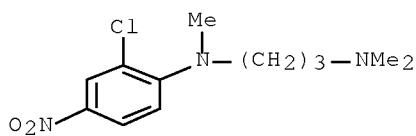
RN 821776-85-6 ZCPLUS

CN 1,2-Ethanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N2,N2-trimethyl- (CA INDEX NAME)

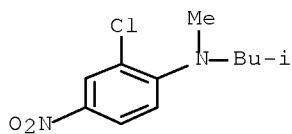
10/560012



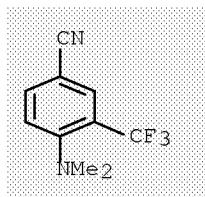
RN 821777-03-1 ZCPLUS  
CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCPLUS  
CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)



IT 71145-96-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; preparation of heteroaryl-containing thiourea derivs.  
as  
inhibitors of herpes viruses)  
RN 71145-96-5 ZCPLUS  
CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/560012

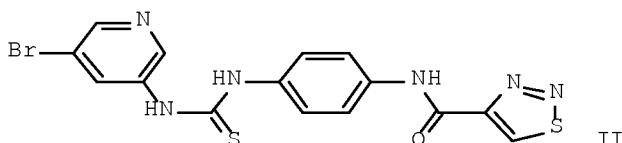
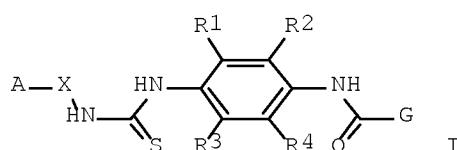
L70 ANSWER 14 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2000:401816 ZCPLUS Full-text  
DOCUMENT NUMBER: 133:30666  
TITLE: Aryl- and heteroaryl-substituted thiourea derivatives useful as inhibitors of herpes viruses  
INVENTOR(S): Bloom, Jonathan David; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; O'Hara, Bryan Mark  
PATENT ASSIGNEE(S): American Home Products Corporation, USA  
SOURCE: PCT Int. Appl., 159 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034268	A1	20000615	WO 1999-US28838	19991206 <--
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BR 9915993	A	20010904	BR 1999-15993	19991206 <--
EP 1137647	A1	20011004	EP 1999-965131	19991206 <--
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HU 2001004611	A3	20021028		
JP 2002531557	T	20020924	JP 2000-586715	19991206 <--
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PRIORITY APPLN. INFO.:			US 1998-207961	A 19981209 <--
			WO 1999-US28838	W 19991206 <--

OTHER SOURCE(S): MARPAT 133:30666

GI



AB Title compds. I and related compds. and their pharmaceutical salts are disclosed [wherein A = heteroaryl; R1-R4 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, cyano; R1R2 or R3R4 = C5-7 aryl fusion; G = aryl or heteroaryl; and X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph or PhCH<sub>2</sub>; n = 1-6]. The compds. are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), and varicella-zoster virus (VZV), as well as (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 35 compds. in 2-4 bioassays. For instance, the pyridine derivative II had an IC<sub>50</sub> of 0.018 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture.

IT 151951-35-8 338981-22-9 821776-85-6

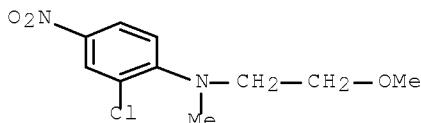
821777-03-1 1098071-56-7

RL: PRPH (Prophetic)

(Aryl- and heteroaryl-substituted thiourea derivatives useful as inhibitors of herpes viruses)

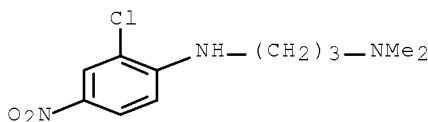
RN 151951-35-8 ZCPLUS

CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



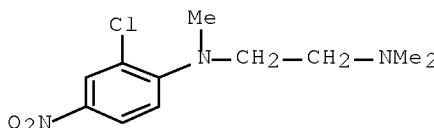
RN 338981-22-9 ZCPLUS

CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



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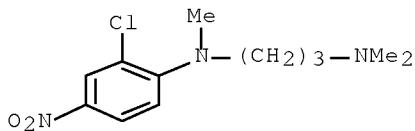
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10/560012

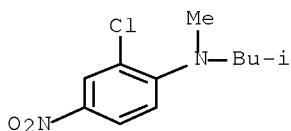
RN 821777-03-1 ZCPLUS

CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCPLUS

CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)



IT 71145-96-5

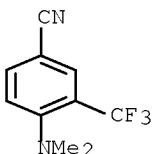
RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of heteroaryl thiourea derivs. as inhibitors

of herpes viruses)

RN 71145-96-5 ZCPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 15 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401809 ZCPLUS Full-text

DOCUMENT NUMBER: 133:30657

TITLE: Heterocyclic carboxamide-containing thiourea derivatives containing a substituted phenylenediamine group, useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi,

Martin Joseph; Dushin, Russell George; Jones, Thomas Richard; Lang, Stanley Albert; Ross, Adma Antonia; Terefenko, Eugene Anthony; O'Hara, Bryan Mark  
American Home Products Corporation, USA

PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 159 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

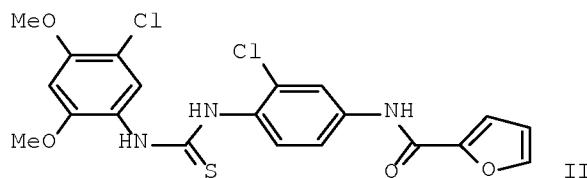
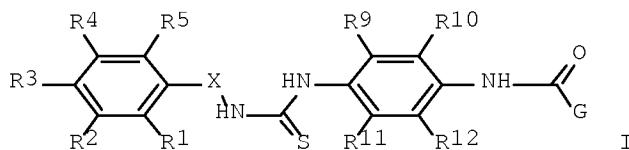
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

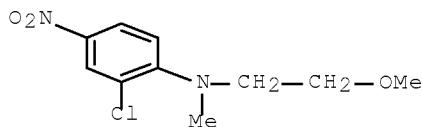
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034261	A2	20000615	WO 1999-US28916	19991206 <--
WO 2000034261	A3	20020131		
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US 6197803	B1	20010306	US 1999-447006	19991122 <--
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HU 2002003405	A2	20030228	HU 2002-3405	19991206 <--
US 6262082	B1	20010717	US 2000-669483	20000925 <--
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PRIORITY APPLN. INFO.:				
		US 1998-208164	A	19981209 <--
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		US 1998-155192P	P	19981209 <--
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		US 1998-208540	A	19981209 <--
		US 1998-208561	A	19981209 <--
		US 1999-444782	A3	19991122 <--
		WO 1999-US28916	W	19991206 <--
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OTHER SOURCE(S): MARPAT 133:30657

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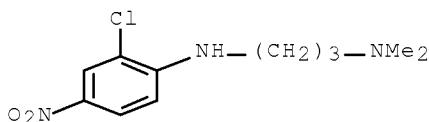
- AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO<sub>2</sub>, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, NR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>), or W-Y-(CH<sub>2</sub>)<sub>n</sub>-Z, provided that at least 1 of R1-R5 ≠ H; or R<sub>2</sub>R<sub>3</sub> or R<sub>3</sub>R<sub>4</sub> form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R<sub>6</sub>, R<sub>7</sub> = H, C1-6 alkyl or perhaloalkyl, or aryl; R<sub>8</sub> = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR<sub>7</sub>R<sub>8</sub> forms 3- to 7-membered heterocycloalkyl; R<sub>9</sub>-R<sub>12</sub> = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R<sub>9</sub>R<sub>10</sub> or R<sub>11</sub>R<sub>12</sub> = C5-7 aryl fusion, provided that at least 1 of R<sub>9</sub>-R<sub>12</sub> ≠ H; W = O, NR<sub>6</sub>, or bond; Y = CO, CO<sub>2</sub>, or bond; Z = C1-4 alkyl, CN, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, OCOR<sub>6</sub>, NR<sub>6</sub>COR<sub>7</sub>, OCONR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, SR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>) or Ph; G = monocyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)<sub>J</sub>; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH<sub>2</sub>; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for 18 compds. in 4 bioassays. For instance, the N-(4-thioureidophenyl)furan-2-carboxamide derivative II had an IC<sub>50</sub> of 0.4 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture, and 0.5 µg/mL against HSV in an ELISA assay.
- IT 151951-35-8 338981-22-9 821776-85-6  
821777-03-1 1098071-56-7
- RL: PRPH (Prophetic)  
(Heterocyclic carboxamide-containing thiourea derivatives containing a substituted phenylenediamine group, useful as inhibitors of herpes viruses)
- RN 151951-35-8 ZCAPLUS
- CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



10/560012

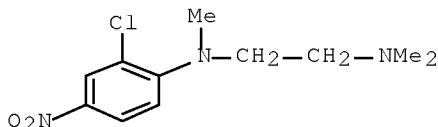
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CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



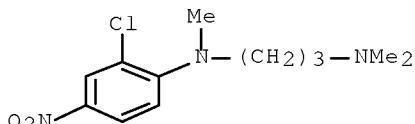
RN 821776-85-6 ZCPLUS

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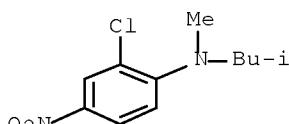
RN 821777-03-1 ZCPLUS

CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCPLUS

CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)



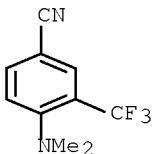
IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of heterocyclic carboxamide-containing and phenylenediamine-containing thiourea derivs. as inhibitors of herpes

10/560012

viruses)  
RN 71145-96-5 ZCPLUS  
CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



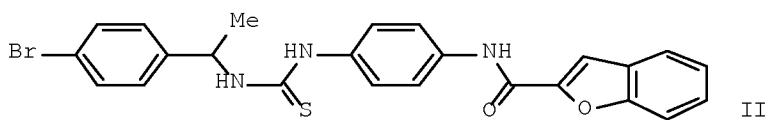
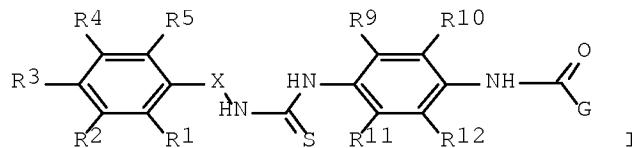
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 16 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2000:401808 ZCPLUS Full-text  
DOCUMENT NUMBER: 133:30588  
TITLE: Alpha-methylbenzyl-containing thiourea derivatives containing a phenylenediamine group, useful as inhibitors of herpes viruses  
INVENTOR(S): Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; Norton, Emily Boucher; Ross, Adma Antonia; O'Hara, Bryan Mark  
PATENT ASSIGNEE(S): American Home Products Corporation, USA  
SOURCE: PCT Int. Appl., 168 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034260	A2	20000615	WO 1999-US28839	19991206 <--
WO 2000034260	A3	20000908		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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BR 9916084	A	20010904	BR 1999-16084	19991206 <--
EP 1137645	A2	20011004	EP 1999-963022	19991206 <--
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JP 2002531555	T	20020924	JP 2000-586707	19991206 <--
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AT 267824	T	20040615	AT 1999-963022	19991206 <--
CN 1165531	C	20040908	CN 1999-814277	19991206 <--
PT 1137645	T	20040930	PT 1999-963022	19991206 <--

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NO 2001002833	A	20010802	NO 2001-2833	20010608 <--
PRIORITY APPLN. INFO.:			US 1998-208902	A 19981209 <--
			WO 1999-US28839	W 19991206 <--

OTHER SOURCE(S): MARPAT 133:30588  
GI



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO<sub>2</sub>, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, NR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>), or W-Y-(CH<sub>2</sub>)<sub>n</sub>-Z, provided that at least 1 of R1-R5 ≠ H; or R<sub>2</sub>R<sub>3</sub> or R<sub>3</sub>R<sub>4</sub> form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R<sub>6</sub>, R<sub>7</sub> = H, C1-6 alkyl or perhaloalkyl, or aryl; R<sub>8</sub> = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR<sub>7</sub>R<sub>8</sub> forms 3- to 7-membered heterocycloalkyl; R<sub>9</sub>-R<sub>12</sub> = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R<sub>9</sub>R<sub>10</sub> or R<sub>11</sub>R<sub>12</sub> = C5-7 aryl fusion; W = O, NR<sub>6</sub>, or bond; Y = CO, CO<sub>2</sub>, or bond; Z = C1-4 alkyl, CN, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, OCOR<sub>6</sub>, NR<sub>6</sub>COR<sub>7</sub>, OCONR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, SR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>) or Ph; G = aryl or fused bicyclic aryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)<sub>J</sub>; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH<sub>2</sub>; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 320 compds. in 1-4 bioassays. For instance, the [[(phenylethyl)thioureido]phenyl]benzofurancarboxamide derivative II had an IC<sub>50</sub> of 1.3 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture, and 0.10 µg/mL against VZV in an ELISA assay.

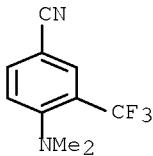
IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of α-methylbenzyl-containing thiourea derivs. as inhibitors of herpes viruses)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 17 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2000:401806 ZCPLUS Full-text  
 DOCUMENT NUMBER: 133:30733  
 TITLE: Heterocyclic carboxamide-containing thiourea derivatives containing a phenylenediamine group, useful as inhibitors of herpes viruses  
 INVENTOR(S): Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Jones, Thomas Richard; Lang, Stanley Albert; Ross, Adma Antonia; Terefenko, Eugene Anthony; O'Hara, Bryan Mark  
 PATENT ASSIGNEE(S): American Home Products Corporation, USA  
 SOURCE: PCT Int. Appl., 188 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 4  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034258	A2	20000615	WO 1999-US28842	19991206 <--
WO 2000034258	A3	20011129		
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CA 2350767	A1	20000615	CA 1999-2350767	19991206 <--
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EP 1144397	A2	20011017	EP 1999-963023	19991206 <--
EP 1144397	A3	20020911		
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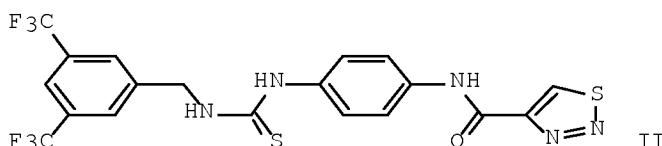
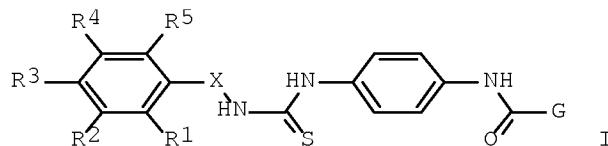
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US 1998-208559	A 19981209 <--
US 1998-150692P	P 19981209 <--
US 1998-150698P	P 19981209 <--
US 1998-155192P	P 19981209 <--
US 1998-155240P	P 19981209 <--
US 1999-444782	A3 19991122 <--
WO 1999-US28842	W 19991206 <--
US 2000-669535	A3 20000926 <--

OTHER SOURCE(S):

MARPAT 133:30733

GI



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO<sub>2</sub>, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, NR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>), or W-Y-(CH<sub>2</sub>)<sub>n</sub>-Z, provided that at least 1 of R1-R5 ≠ H; or R<sub>2</sub>R<sub>3</sub> or R<sub>3</sub>R<sub>4</sub> form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R<sub>6</sub>, R<sub>7</sub> = H, C1-6 alkyl or perhaloalkyl, or aryl; R<sub>8</sub> = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR<sub>7</sub>R<sub>8</sub> forms 3- to 7-membered heterocycloalkyl; W = O, NR<sub>6</sub>, or bond; Y = CO, CO<sub>2</sub>, or bond; Z = C1-4 alkyl, CN, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, OCOR<sub>6</sub>, NR<sub>6</sub>COR<sub>7</sub>, OCONR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, SR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>) or Ph; G = monocyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)<sub>J</sub>; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH<sub>2</sub>; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 350 compds. in 1-4 bioassays. For instance, the thioureidophenylthiadiazolecarboxamide derivative II had an IC<sub>50</sub> of 0.0011 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture.

IT 151951-35-8 338981-22-9 821776-85-6  
821777-03-1 1098071-56-7

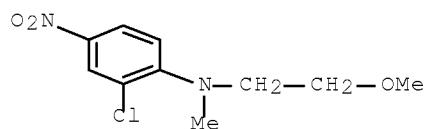
RL: PRPH (Prophetic)

(Heterocyclic carboxamide-containing thiourea derivatives containing a phenylenediamine group, useful as inhibitors of herpes viruses)

RN 151951-35-8 ZCAPLUS

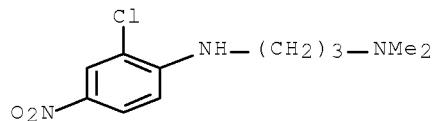
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10/560012



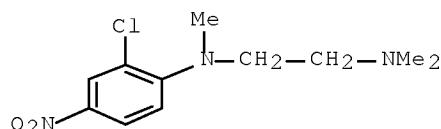
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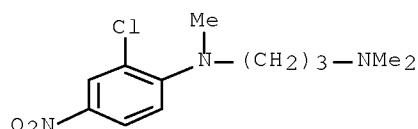
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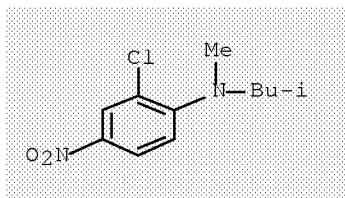
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RN 1098071-56-7 ZCPLUS

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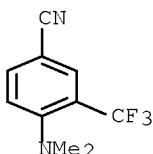
IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (starting material; preparation of heterocyclic carboxamide-containing thiourea

derivs. as inhibitors of herpes viruses)

RN 71145-96-5 ZCPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 18 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401786 ZCPLUS Full-text

DOCUMENT NUMBER: 133:30587

TITLE: Benzamide-containing aryl thiourea derivatives useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; Norton, Emily Boucher; Ross, Adma Antonia; O'Hara, Bryan Mark

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: PCT Int. Appl., 169 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

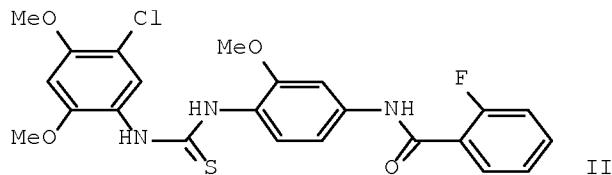
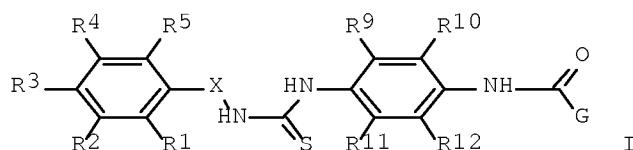
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OTHER SOURCE(S): MARPAT 133:30587  
GI



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO<sub>2</sub>, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, NR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>), or W-Y-(CH<sub>2</sub>)<sub>n</sub>-Z, provided that at least 1 of R1-R5 ≠ H; or R<sub>2</sub>R<sub>3</sub> or R<sub>3</sub>R<sub>4</sub> form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R<sub>6</sub>, R<sub>7</sub> = H, C1-6 alkyl or perhaloalkyl, or aryl; R<sub>8</sub> = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR<sub>7</sub>R<sub>8</sub> forms 3- to 7-membered heterocycloalkyl; R<sub>9</sub>-R<sub>12</sub> = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R<sub>9</sub>R<sub>10</sub> or R<sub>11</sub>R<sub>12</sub> = C5-7 aryl fusion, provided that at least 1 of R<sub>9</sub>-R<sub>12</sub> ≠ H; W = O, NR<sub>6</sub>, or bond; Y = CO, CO<sub>2</sub>, or bond; Z = C1-4 alkyl, CN, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, OCOR<sub>6</sub>, NR<sub>6</sub>COR<sub>7</sub>, OCONR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, SR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>) or Ph; G = aryl or fused bicyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)<sub>J</sub>; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH<sub>2</sub>; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 75 compds. in 2-4 bioassays. For instance, the thioureidophenylbenzamide derivative II had an IC<sub>50</sub> of 1.5 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture, and 0.04 µg/mL against HSV in an ELISA assay.

IT 151951-35-8 338981-22-9 821776-85-6

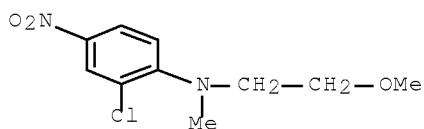
821777-03-1 1098071-56-7

RL: PRPH (Prophetic)

(Benzamide-containing aryl thiourea derivatives useful as inhibitors of herpes viruses)

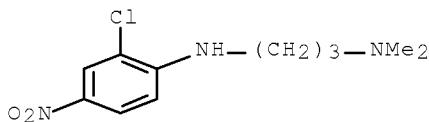
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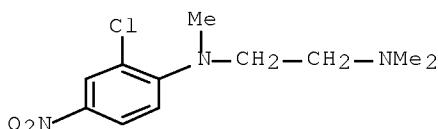


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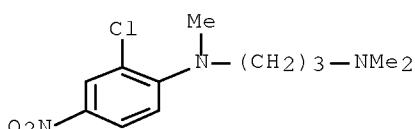
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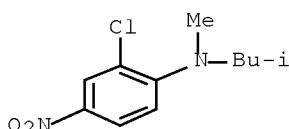
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RN 821777-03-1 ZCPLUS  
CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCPLUS  
CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)



IT 71145-96-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; preparation of benzamide-containing aryl thiourea)

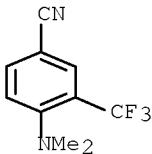
10/560012

derivs. as

inhibitors of herpes viruses)

RN 71145-96-5 ZCPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 19 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401785 ZCPLUS Full-text

DOCUMENT NUMBER: 133:30586

TITLE: Acetamide and substituted acetamide-containing aryl thiourea derivatives useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; O'Hara, Bryan Mark

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

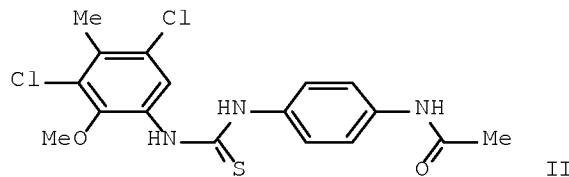
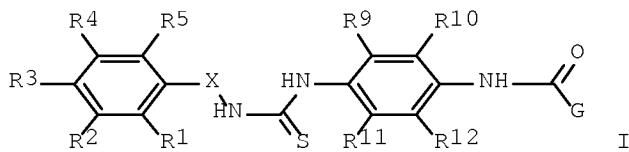
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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NO 2001002834	A	20010807	NO 2001-2834	20010608 <--
PRIORITY APPLN. INFO.:			US 1998-208316	A 19981209 <--
			WO 1999-US28844	W 19991206 <--

OTHER SOURCE(S):  
GI

MARPAT 133:30586



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO<sub>2</sub>, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, NR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>), or W-Y-(CH<sub>2</sub>)<sub>n</sub>-Z, provided that at least 1 of R1-R5 ≠ H; or R<sub>2</sub>R<sub>3</sub> or R<sub>3</sub>R<sub>4</sub> form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R<sub>6</sub>, R<sub>7</sub> = H, C1-6 alkyl or perhaloalkyl, or aryl; R<sub>8</sub> = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR<sub>7</sub>R<sub>8</sub> forms 3- to 7-membered heterocycloalkyl; R<sub>9</sub>-R<sub>12</sub> = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R<sub>9</sub>R<sub>10</sub> or R<sub>11</sub>R<sub>12</sub> = C5-7 aryl fusion; W = O, NR<sub>6</sub>, or bond; Y = CO, CO<sub>2</sub>, or bond; Z = C1-4 alkyl, CN, CO<sub>2</sub>R<sub>6</sub>, COR<sub>6</sub>, CONR<sub>7</sub>R<sub>8</sub>, OCOR<sub>6</sub>, NR<sub>6</sub>COR<sub>7</sub>, OCONR<sub>6</sub>, OR<sub>6</sub>, SR<sub>6</sub>, SOR<sub>6</sub>, SO<sub>2</sub>R<sub>6</sub>, SR<sub>6</sub>N(R<sub>7</sub>R<sub>8</sub>), N(R<sub>7</sub>R<sub>8</sub>) or Ph; G = C1-6 alkyl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)<sub>J</sub>; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH<sub>2</sub>; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 160 compds. in 4 bioassays. For instance, the thioureidophenylacetamide derivative II had an IC<sub>50</sub> of 0.8 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture, and 2 µg/mL against HSV in an ELISA assay.

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821777-03-1 1098071-56-7

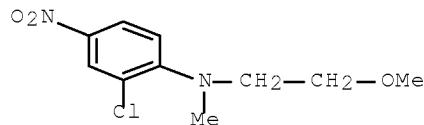
RL: PRPH (Prophetic)

(Acetamide and substituted acetamide-containing aryl thiourea derivatives useful as inhibitors of herpes viruses)

RN 151951-35-8 ZCAPLUS

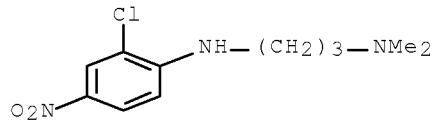
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10/560012



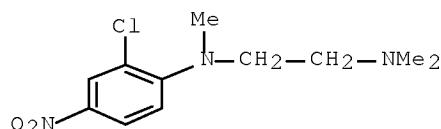
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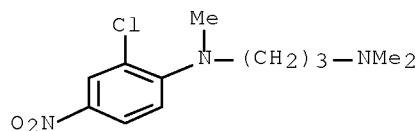
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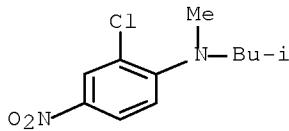
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RN 1098071-56-7 ZCPLUS

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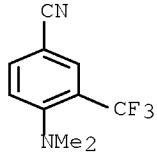


IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (starting material; preparation of acetamide-containing aryl thiourea derivs. as  
 inhibitors of herpes viruses)

RN 71145-96-5 ZCPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 20 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2000:259962 ZCPLUS Full-text  
 DOCUMENT NUMBER: 132:283910  
 TITLE: Agent and method for dyeing fibers  
 INVENTOR(S): Braun, Hans-Juergen; Semadeni, Pascal Andre  
 PATENT ASSIGNEE(S): Wella Aktiengesellschaft, Germany  
 SOURCE: PCT Int. Appl., 56 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1037593	A1	20000927	EP 1999-944624	19990908 <--
EP 1037593	B1	20040204		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9906871	A	20001017	BR 1999-6871	19990908 <--
JP 2002527369	T	20020827	JP 2000-575472	19990908 <--
AT 258782	T	20040215	AT 1999-944624	19990908 <--
ES 2214882	T3	20040916	ES 1999-944624	19990908 <--
US 6379400	B1	20020430	US 2000-581367	20000612 <--

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PRIORITY APPLN. INFO.:

DE 1998-19847192

A 19981013 <--

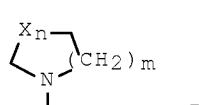
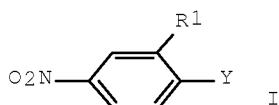
WO 1999-EP6601

W 19990908 <--

OTHER SOURCE(S):

MARPAT 132:283910

GI



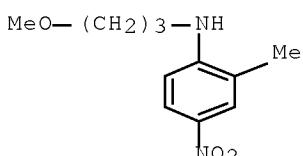
AB Direct dyes for fibers, especially hair, which contain 4-nitrophenylamine derivs. I [R1 = H, C1-4 alkyl; Y = II, cycloalkyl, NR2R3, (CH2)zOR4;  $\geq 1$  of R2, R3  $\neq$  H; R4 = C1-4 alkyl; X = N, O; m = 1-3; n = 0, 1; z = 1-6] are prepared which are readily water soluble, fast towards light, friction, permanent waving, and perspiration, and produce a brilliant yellow coloration. I can be used in conjunction with other direct dyes or with oxidative dyes. Thus, 1-fluoro-4-nitrobenzene reacted with 1-amino-2-methoxyethane to form N-(2-methoxyethyl)-4-nitrophenylamine (III). A composition containing III 0.49, iso-PrOH 10.00, 28% aqueous lauryl alc. diglycol ether sulfate Na salt 10.00, and H2O to 100.00 g was adjusted to pH 5 or 8 and applied to bleached hair at 40° for 40 min to produce an intense lemon-yellow color at either pH.

IT 263902-65-4P

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(agent and method for dyeing fibers)

RN 263902-65-4 ZCPLUS

CN Benzenamine, N-(3-methoxypropyl)-2-methyl-4-nitro- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 21 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:125899 ZCPLUS Full-text

DOCUMENT NUMBER: 128:250295

ORIGINAL REFERENCE NO.: 128:49441a, 49444a

TITLE: Pattern recognition corresponding analysis of powder frequency doubling effect of the nitrobenzene derivatives

AUTHOR(S): Yang, Rongsheng; Chen, Jiangzhong; Zhang, Hanhui

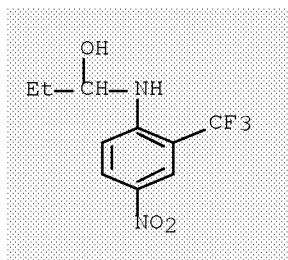
CORPORATE SOURCE: Department of Chemistry, Fuzhou University, Fuzhou, 350002, Peop. Rep. China

SOURCE: Fuzhou Daxue Xuebao, Ziran Kexueban (1997), 25(3), 95-98

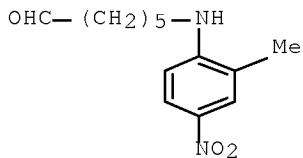
CODEN: FDXKEN; ISSN: 1000-2243

10/560012

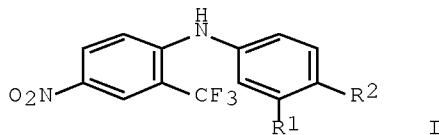
PUBLISHER: Fuzhou Daxue Xuebao Bianjibu  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese  
AB The relationship between the structure and powder frequency doubling effect was studied by pattern recognition corresponding anal. method to avoid space group problems. Two groups of binding relationships were formulated, which can predict crystals with higher powder frequency doubling effect. Path for mol. engineering and crystal engineering was discussed.  
IT 204931-24-8  
RL: PRP (Properties)  
(pattern recognition corresponding anal. of powder frequency doubling effect of nitrobenzene derivative)  
RN 204931-24-8 ZCPLUS  
CN 1-Propanol, 1-[(4-nitro-2-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



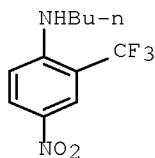
L70 ANSWER 22 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1998:89624 ZCPLUS Full-text  
DOCUMENT NUMBER: 128:192539  
ORIGINAL REFERENCE NO.: 128:38035a, 38038a  
TITLE: The reactivity of nitrophenyl-substituted cyclic amines in dehydrogenations  
AUTHOR(S): Moehrle, H.; Mehrens, J.  
CORPORATE SOURCE: Institut Pharmazeutische Chemie,  
Heinrich-Heine-Universitaet, Duesseldorf, D-40225,  
Germany  
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences  
(1998), 53(1), 37-48  
CODEN: ZNBSEN; ISSN: 0932-0776  
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
OTHER SOURCE(S): CASREACT 128:192539  
AB 1-(4-Nitrophenyl)-substituted piperidine and perhydroazepine were inert to Hg(II)-EDTA, while the corresponding  $\alpha$ -pipercoline gave an amino ketone with ring cleavage. However, the corresponding 2-nitrophenyl compds. reacted to give a 2-piperidinone, an aminopentanal, and an aminohexanone, resp. By an addnl. substituent in 2'-position the 4-nitro compds. underwent dehydrogenation too. With a Me group resulted a pattern analogous to 2-nitro products. A neighboring CH<sub>2</sub>OH function enhanced the reaction with formation of benzoxazines and if possible their further oxidized derivs., hydroxy lactams.  
IT 203510-10-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(dehydrogenation of nitrophenyl-substituted cyclic amines)  
RN 203510-10-5 ZCPLUS  
CN Hexanal, 6-[(2-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



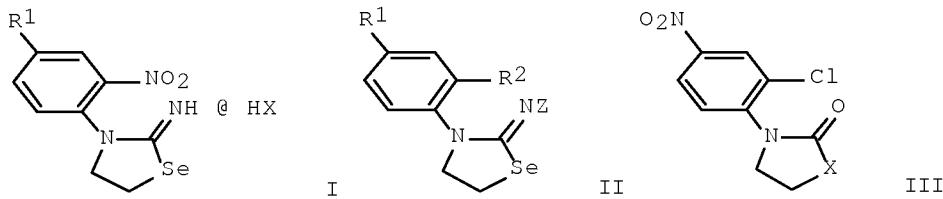
L70 ANSWER 23 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1996:561104 ZCPLUS Full-text  
 DOCUMENT NUMBER: 125:275309  
 ORIGINAL REFERENCE NO.: 125:51485a,51488a  
 TITLE: Synthesis of substituted diphenylamines under phase transfer catalysis  
 AUTHOR(S): Durantini, Edgardo N.; Chiacchiera, Stella M.; Silber, Juana J.  
 CORPORATE SOURCE: Dep. Quim. Fis., Univ. Nacl. Rio Cuarto, Rio Cuarto, 5800, Argent.  
 SOURCE: Synthetic Communications (1996), 26(20), 3849-3858  
 CODEN: SYNCVA; ISSN: 0039-7911  
 PUBLISHER: Dekker  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 125:275309  
 GI



AB A convenient procedure for the synthesis of N-[(trifluoromethyl)nitrophenyl] substituted anilines, e.g., I (R1 = H, R2 = NO<sub>2</sub>; R1 = NO<sub>2</sub>, R2 = H; R1 = H, R2 = cyano), by means of a chloro-substitution reaction under conditions of phase-transfer catalysis (PTC) is reported. This method provides a general procedure for the synthesis of diphenylamines bearing electron-withdrawing groups in both aromatic rings.  
 IT 175873-18-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of diphenylamines under phase transfer catalysis)  
 RN 175873-18-4 ZCPLUS  
 CN Benzenamine, N-butyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



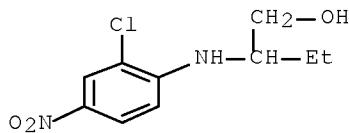
L70 ANSWER 24 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1996:426976 ZCPLUS Full-text  
 DOCUMENT NUMBER: 125:195846  
 ORIGINAL REFERENCE NO.: 125:36687a, 36690a  
 TITLE: Synthesis, some reactions and anti-ulcer activity of some 2-amino-3-(substituted phenyl)selenazolidines  
 AUTHOR(S): Hornyak, Gyula; Feller, Antal; Lempert, Karoly  
 CORPORATE SOURCE: Res. Group Alkaloid Chem., Hungarian Academy Sci., Budapest, H-1521, Hung.  
 SOURCE: ACH - Models in Chemistry (1995), 132(6), 871-885  
 CODEN: ACMCEI; ISSN: 1217-8969  
 PUBLISHER: Akademiai Kiado  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 125:195846  
 GI



AB 2-Imino-3-(substituted phenyl)selenazolidine salts, e.g., I ( $R_1 = H, NO_2, CF_3$ ,  $X = Cl, Br$ ), were prepared (1) by acid induced ring closure of N-(2-selenocyanatoethyl)anilines, or (2) by fusion of anilines with 2-bromoethylselenocyanate. E.g.,  $2-NO_2C_6H_4NHCH_2CH_2SeCN$  is refluxed in dioxane the presence of ethanesulfonic acid to give I ( $R_1 = H$ ,  $HX = HO_3SEt$ ) in 93% yield. Diselenide, e.g.,  $(ArNHCH_2CH_2Se)_2$ , formation accompanying the syntheses according to Method 1 above was successfully suppressed. Some N-substituted derivs. (e.g., II,  $R_1 \neq R_2 = Cl, NO_2$ ,  $Z = CHO, Ac, CONHPr, SO_2Et$ ) of selenazolidines I, as well as 3-aryl-selenazolidin-2-one III ( $X = Se$ ), and its thiazolidinone analog III ( $X = S$ ), were also prepared. The gastroprotective (antiulcer) activity of some of I, II and III is reported.

IT 180691-77-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and methylsulfonylation in the synthesis of amino(substituted phenyl)selenazolidines as antiulcer agents)

RN 180691-77-4 ZCPLUS  
 CN 1-Butanol, 2-[(2-chloro-4-nitrophenyl)amino]- (CA INDEX NAME)



L70 ANSWER 25 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:259463 ZCPLUS Full-text

DOCUMENT NUMBER: 124:288977

ORIGINAL REFERENCE NO.: 124:53579a, 53582a

TITLE: Preparation of nitroarylamines

INVENTOR(S): Jautelat, Manfred

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 695737	A1	19960207	EP 1995-111426	19950720 <--
EP 695737	B1	19970618		
R: BE, DE, FR, GB, IT, NL				
DE 4427249	A1	19960208	DE 1994-4427249	19940802 <--
US 5684203	A	19971104	US 1995-504034	19950726 <--
CA 2154965	A1	19960203	CA 1995-2154965	19950728 <--
JP 08059571	A	19960305	JP 1995-211399	19950728 <--
PRIORITY APPLN. INFO.:			DE 1994-4427249	A 19940802 <--

OTHER SOURCE(S): CASREACT 124:288977; MARPAT 124:288977

AB RHNZ(Xn)NO<sub>2</sub> [R = H, (cyclo)alkyl, alkenyl, aryl, etc.; X = halo, cyano, alkyl, alkoxy, etc.; Z = (n+2)-valent (hetero)aryl group; n = 0-3] were prepared by amination of Z(Xn)NO<sub>2</sub> [Z = (n+1)-valent (hetero)aryl group] by (RNH)<sub>2</sub>CY (Y = O or S) in the presence of a base, O, and a dipolar solvent. Thus, 3-(F<sub>3</sub>C)C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub> was heated 4h at 50° with (MeNH)<sub>2</sub>CO in DMSO containing NaOH and with air sparging to give 100% N-methyl-4-nitro-2-trifluoromethylaniline.

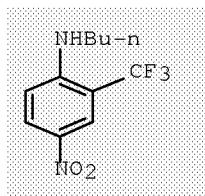
IT 175873-18-4P, N-Butyl-4-nitro-2-trifluoromethylaniline

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of nitroarylamines)

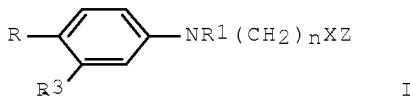
RN 175873-18-4 ZCPLUS

CN Benzenamine, N-butyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 26 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1995:169712 ZCPLUS Full-text  
 DOCUMENT NUMBER: 122:31106  
 ORIGINAL REFERENCE NO.: 122:6139a,6142a  
 TITLE: Preparation of p-phenylenediamines  
 INVENTOR(S): Urano, Fumiyoshi; Kimura, Takahiro; Kametani, Miki  
 PATENT ASSIGNEE(S): Wako Pure Chem Ind Ltd, Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06219997	A	19940809	JP 1993-28593	19930125 <--
PRIORITY APPLN. INFO.:			JP 1993-28593	19930125 <--
OTHER SOURCE(S):	CASREACT 122:31106; MARPAT 122:31106			
GI				



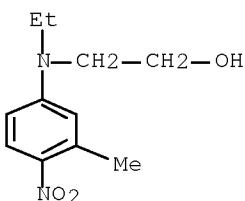
AB The title compds. [I; R = NH<sub>2</sub>; R<sub>1</sub> = C<sub>1</sub>-3 alkyl; R<sub>3</sub> = H, C<sub>1</sub>-3 alkyl, C<sub>1</sub>-3 alkoxy; X = O, NH; Z = H, COR<sub>4</sub>, SO<sub>2</sub>R<sub>4</sub>; R<sub>4</sub> = C<sub>1</sub>-3 alkyl, (alkyl)phenyl; n = 1-3], useful as intermediates for azo dyes, pharmaceuticals, and agrochems. and photog. developers (no data), are prepared by nitration of I [R = H; Z = YR<sub>2</sub>; R<sub>2</sub> = C<sub>1</sub>-3 alkyl, (alkyl)phenyl; Y = CO, SO<sub>2</sub>], treatment with H<sub>2</sub>O or alkaline aqueous solns., and reduction of the resulting I (R = NO<sub>2</sub>; Z = H, COR<sub>4</sub>, SO<sub>2</sub>R<sub>4</sub>). I (R = H, R<sub>1</sub> = Et, R<sub>3</sub> = Me, XZ = OAc, n = 2) (preparation given) was nitrated by HNO<sub>3</sub> and H<sub>2</sub>SO<sub>4</sub> at -5 to 0° for 3 h and treated with aqueous NaOH in MeOH at 25-30° for 2 h to give 99% I (R = NO<sub>2</sub>, R<sub>1</sub> = Et, R<sub>3</sub> = Me, XZ = OH, n = 2), which was reduced by H with Pd/C in EtOH at 25-35° for 6 h to give 95% sulfate salt of I (R = NH<sub>2</sub>, R<sub>1</sub> = Et, R<sub>3</sub> = Me, XZ = OH, n = 2).

IT 52177-13-6P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of phenylenediamines from anilines via nitroanilines)

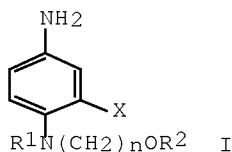
RN 52177-13-6 ZCPLUS

CN Ethanol, 2-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



L70 ANSWER 27 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1994:77020 ZCPLUS Full-text  
 DOCUMENT NUMBER: 120:77020  
 ORIGINAL REFERENCE NO.: 120:13849a,13852a  
 TITLE: Preparation of N-alkoxyalkyl p-phenylenediamine  
 developers for oxidative hair dyes  
 INVENTOR(S): Rose, David; Lieske, Edgar; Hoeffkes, Horst  
 PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany  
 SOURCE: Ger. Offen., 7 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4205329	A1	19930826	DE 1992-4205329	19920221 <--
WO 9316679	A1	19930902	WO 1993-EP351	19930213 <--
W: JP, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			DE 1992-4205329	A 19920221 <--
OTHER SOURCE(S):		MARPAT	120:77020	
GI				



AB Title compds. (I; R1, R2 = alkyli; X = H, halo; n = 2-4), were prepared Thus, 4-FC6H4NO2, CaCO3, and MeNHCH2CH2OMe were refluxed in acetone to give 4-O2NC6H4NMeCH2CH2OMe, which was hydrogenated followed by salification with HCl to give 4-H2NC6H4NMeCH2CH2OMe.2HCl. This developer together with 2-chloro-3-amino-6methylphenol coupler and 3% H2O3 oxidizer gave a blue-black color to gray hair.

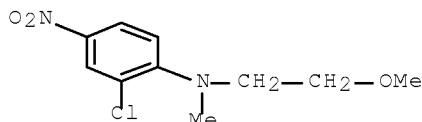
IT 151951-35-8P

RL: PREP (Preparation)

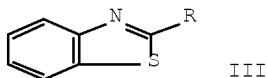
(prepare of, as intermediate for developer for oxidative hair dyes)

RN 151951-35-8 ZCPLUS

CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)

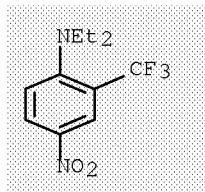


L70 ANSWER 28 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1991:247193 ZCPLUS Full-text  
 DOCUMENT NUMBER: 114:247193  
 ORIGINAL REFERENCE NO.: 114:41737a, 41740a  
 TITLE: Acyclic tertiary amines as nucleophiles in substitution reactions of aromatic and heteroaromatic halides  
 AUTHOR(S): Matsumoto, Kiyoshi; Hashimoto, Shiro; Otani, Shinichi  
 CORPORATE SOURCE: Coll. Lib. Arts Sci., Kyoto Univ., Kyoto, 606, Japan  
 SOURCE: Journal of the Chemical Society, Chemical Communications (1991), (5), 306-7  
 CODEN: JCCCAT; ISSN: 0022-4936  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Even acyclic tertiary amines such as Et<sub>3</sub>N, Pr<sub>3</sub>N and Bu<sub>3</sub>N, which have been believed to be inert to aromatic and heteroarom. halides, underwent SNAr reactions with aromatic and heteroarom. halides to give the dialkylamino derivs. via an addition-elimination mechanism; in the case of monocyclic amines like N-methylpyrrolidine (I) and N-methylpiperidine (II) the dealkylation being regioselective. Thus, the reaction of 2-chlorobenzothiazole III (R = Cl) with I and II gave 92-96% III (R = pyrrolidino, piperidino) resp.

IT 25900-35-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 25900-35-0 ZCPLUS  
 CN Benzenamine, N,N-diethyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



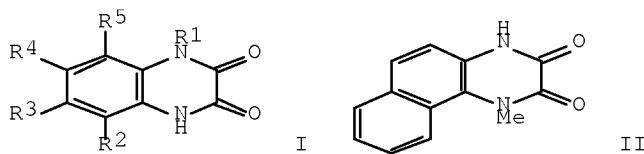
L70 ANSWER 29 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1989:632859 ZCPLUS Full-text  
 DOCUMENT NUMBER: 111:232859

10/560012

ORIGINAL REFERENCE NO.: 111:38689a, 38692a  
 TITLE: Preparation and testing of  
 2,3(1H,4H)-quinoxalinediones as neuroleptics  
 INVENTOR(S): Honore, Tage; Jacobsen, Poul; Elmelund, Flemming;  
 Naerum, Lars  
 PATENT ASSIGNEE(S): Aktieselskabet Ferrosan, Den.  
 SOURCE: Eur. Pat. Appl., 28 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 315959	A2	19890517	EP 1988-118592	19881108 <--
EP 315959	A3	19891227		
EP 315959	B1	19940302		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 164317	C	19921102	DK 1987-5862	19871110 <--
NO 8804729	A	19890511	NO 1988-4729	19881024 <--
NO 179551	B	19960722		
NO 179551	C	19961030		
CA 1321587	C	19930824	CA 1988-582104	19881103 <--
DK 8806206	A	19890511	DK 1988-6206	19881108 <--
DK 164317	B	19920609		
ZA 8808367	A	19890830	ZA 1988-8367	19881108 <--
US 4948794	A	19900814	US 1988-268939	19881108 <--
AT 102192	T	19940315	AT 1988-118592	19881108 <--
ES 2061606	T3	19941216	ES 1988-118592	19881108 <--
AU 8824949	A	19890511	AU 1988-24949	19881109 <--
AU 618766	B2	19920109		
FI 8805151	A	19890511	FI 1988-5151	19881109 <--
FI 100181	B1	19971015		
JP 01153680	A	19890615	JP 1988-282621	19881110 <--
JP 2721520	B2	19980304		
KR 9711279	B1	19970709	KR 1988-14744	19881110 <--
US 5026704	A	19910625	US 1989-456325	19891226 <--
NO 9603412	A	19890511	NO 1996-3412	19960815 <--
NO 307252	B1	20000306		
PRIORITY APPLN. INFO.:			DK 1987-5862	A 19871110 <--
			DK 1988-1422	A 19880316 <--
			NO 1988-4729	A 19881024 <--
			EP 1988-118592	A 19881108 <--
			US 1988-268939	A1 19881108 <--

OTHER SOURCE(S): MARPAT 111:232859  
 GI



10/560012

AB The title compds. [I; R1 = C3-8 cycloalkyl, aryl, aralkyl, (un)substituted C1-12 alkyl; R2-R5 = H, CF<sub>3</sub> C1-4 alkoxy, cyano, halo, NO<sub>2</sub>; R2R3, R4R5 = atoms to complete an (un)substituted, fused aromatic ring; when R1 = Me, R3 ≠ CF<sub>3</sub>, MeO, Br, Cl, NO<sub>2</sub>] were prepared as neurotransmitter antagonists, especially at NMDA (N-methyl-D-aspartate), quisqualate, and kainate receptors. I are useful as tranquilizers. 2-Bromo-6-methoxynaphthalene was nitrated to give 73% 6-bromo-2-methoxy-1-nitronaphthalene which was treated with MeNH<sub>2</sub> in DMF to give 96% 6-bromo-N-methyl-1-nitro-2-naphthylamine. The latter was hydrogenated over Pd-C and the product was refluxed with (CO<sub>2</sub>H)2.2H<sub>2</sub>O in 4 M HCl to give 92% benzoquinolinedione II. II inhibited AMPA ( $\alpha$ -amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid) binding to quisqualate receptors in rat cerebral cortical membrane preps. with an IC<sub>50</sub> of 0.42 µg/mL.

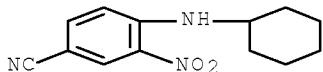
IT 28096-55-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of tranquilizers)

RN 28096-55-1 ZCPLUS

CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)



L70 ANSWER 30 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:486773 ZCPLUS Full-text

DOCUMENT NUMBER: 111:86773

ORIGINAL REFERENCE NO.: 111:14447a,14450a

TITLE: Organic crystals for nonlinear optics: molecular engineering of non-centrosymmetric crystal structures  
Nicoud, J. F.

AUTHOR(S): Nicoud, J. F.  
CORPORATE SOURCE: Inst. Phys. Chim. Mater., Inst. Charles Sadron,  
Strasbourg, F-67083, Fr.

SOURCE: Special Publication - Royal Society of Chemistry  
(1989), 69(Org. Mater. Non-linear Opt.), 157-62  
CODEN: SROCD0; ISSN: 0260-6291

DOCUMENT TYPE: Journal

LANGUAGE: English

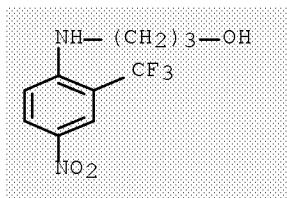
AB Some recent results are presented concerning the use of chirality as an efficient strategy for the tentative control of non-centrosymmetry in organic crystals. In addition to the classical nitro-Ph or nitro-pyridine derivs., some new conjugated chains were studied, such as chalcone and 2-benzylidene-1,3-indanedione derivs. The nonlinear optical properties of these new materials were tested by 2nd-harmonic generation on crystalline powders, at 1.06 or 1.32 µm.

IT 115416-49-4 115416-50-7

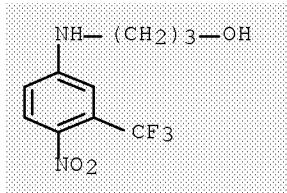
RL: PROC (Process)  
(second-harmonic generation of)

RN 115416-49-4 ZCPLUS

CN 1-Propanol, 3-[{[4-nitro-2-(trifluoromethyl)phenyl]amino}- (CA INDEX NAME)

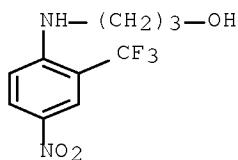


RN 115416-50-7 ZCPLUS  
 CN 1-Propanol, 3-[[4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

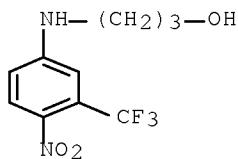


L70 ANSWER 31 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1988:463796 ZCPLUS Full-text  
 DOCUMENT NUMBER: 109:63796  
 ORIGINAL REFERENCE NO.: 109:10551a,10554a  
 TITLE: Molecular and crystal engineering for organic nonlinear optical materials  
 AUTHOR(S): Nicoud, J. F.  
 CORPORATE SOURCE: ESPCI, UA, CNRS, Paris, 75231, Fr.  
 SOURCE: Molecular Crystals and Liquid Crystals (1988), 156(Pt. A), 257-68  
 CODEN: MCLCA5; ISSN: 0026-8941  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Nonlinear optical crystals are attractive due to their potential applications in optical signal processing. Several strategies were investigated to get efficient organic nonlinear optical crystals having enhanced quadratic responses and high efficiencies for 2nd harmonic generation. One chooses mols. with high mol. hyperpolarizability,  $\beta$ . Typical mols. possess a highly delocalized  $\pi$ -electron system bearing a donor and an acceptor group in such positions that an intramol. charge transfer occurs. These mols. must be assembled in an optimized acentric fashion to get a material having a high 2nd order elec. susceptibility,  $\chi(2)$ . The use of chirality to ensure noncentrosym. crystal structures, extra polar groups to influence dipole-dipole interactions, push-pull N-oxide bonds and H bonding were satisfactory strategies to get some of the most efficient organic crystals for nonlinear optics.  
 IT 115416-49-4P 115416-50-7P  
 RL: PREP (Preparation)  
 (preparation of, in mol. and crystal engineering for organic nonlinear optical materials)  
 RN 115416-49-4 ZCPLUS  
 CN 1-Propanol, 3-[[4-nitro-2-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

10/560012



RN 115416-50-7 ZCPLUS  
CN 1-Propanol, 3-[(4-nitro-3-(trifluoromethyl)phenyl)amino]- (CA INDEX NAME)



L70 ANSWER 32 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1982:103817 ZCPLUS Full-text  
DOCUMENT NUMBER: 96:103817  
ORIGINAL REFERENCE NO.: 96:17037a,17040a  
TITLE: Nitrating anilides  
INVENTOR(S): Peer, Lydia; Mayer, Joseph  
PATENT ASSIGNEE(S): Schering Corp., USA  
SOURCE: U.S., 4 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

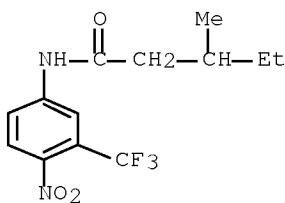
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4302599	A	19811124	US 1979-73838	19790910 <--
PRIORITY APPLN. INFO.:			US 1979-73838	19790910 <--

OTHER SOURCE(S): MARPAT 96:103817

AB Meta-substituted N-acylanilines reacted with HNO<sub>3</sub>-oleum mixts. at between -20 and +50° to yield p-nitro-N-acylanilines. Thus, 3-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>NHCOCHMe<sub>2</sub> was added slowly to oleum at .apprx.5°, 90% HNO<sub>3</sub> was added dropwise, and the mixture was stirred 2 h at .apprx.5° to give 3,4-F<sub>3</sub>C(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>NHCOCHMe<sub>2</sub>. The products are useful as bactericides, herbicides, and antiandrogenic agents (no data).

IT 80945-17-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 80945-17-1 ZCPLUS  
CN Pentanamide, 3-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

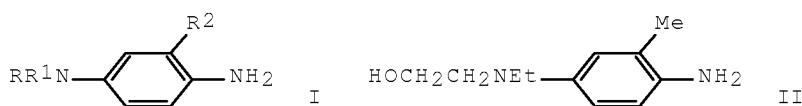


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 33 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1981:586828 ZCPLUS Full-text  
 DOCUMENT NUMBER: 95:186828  
 ORIGINAL REFERENCE NO.: 95:31169a,31172a  
 TITLE: N,N-Disubstituted p-phenylenediamine derivatives  
 INVENTOR(S): Wollemann, Bruno; Haertner, Harrmut; Bardonne, Hans  
 PATENT ASSIGNEE(S): Merck Patent G.m.b.H. , Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 17 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2951100	A1	19810702	DE 1979-2951100	19791219 <--
DE 2951100	C2	19830210		
FR 2471967	A1	19810626	FR 1980-26664	19801216 <--
FR 2471967	B1	19840316		
GB 2065657	A	19810701	GB 1980-40329	19801217 <--
GB 2065657	B	19830824		
JP 56095152	A	19810801	JP 1980-179116	19801219 <--
JP 63053981	B	19881026		
US 4474987	A	19841002	US 1982-365131	19820405 <--
PRIORITY APPLN. INFO.:			DE 1979-2951100	A 19791219 <--
			US 1980-218249	A1 19801219 <--

OTHER SOURCE(S): MARPAT 95:186828  
 GI



AB Title phenylenediamines I (R = C1-6 alkyl; R1 = C1-6 alkyl, sulfo- or alkylsulfonamidoalkyl; R2 = H, alkyl), useful as developers for color photog. (no data), were prepared Thus, 3-MeC6H4NETCH2CH2OH was nitrosated with Me2CHONO, and the nitroso compound hydrogenated over Pd/C to give II (as the sulfate monohydrate).

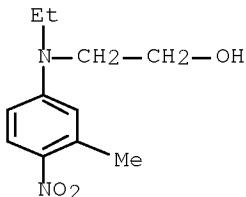
10/560012

IT 52177-13-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrogenation of)

RN 52177-13-6 ZCPLUS

CN Ethanol, 2-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



L70 ANSWER 34 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1981:575793 ZCPLUS Full-text

DOCUMENT NUMBER: 95:175793

ORIGINAL REFERENCE NO.: 95:29269a,29272a

TITLE: Aniline derivatives as anti-testosterone drugs

PATENT ASSIGNEE(S): Scherico Ltd., Switz.

SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

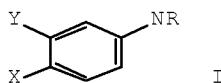
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56063916	A	19810530	JP 1980-87231	19800626 <--
JP 56049884	B	19811125	JP 1971-45301	19710624 <--
JP 58140052	A	19830819	JP 1982-161540	19820916 <--
PRIORITY APPLN. INFO.:			JP 1971-45301	A 19710624 <--
			DE 1971-2130450	A 19710619 <--
			JP 1980-87231	19800626 <--

GI



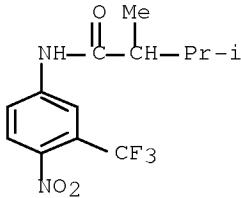
I

AB I (R = H or C1-4 alkyl, X = NO2 or Cl, Y = H, Me, CF3, F, or Cl, Z = H, COCHMe2, or other acyl groups) are synthesized as testosterone inhibitors. Thus, N-(isobutyryl)-4-nitro-3-trifluoromethylaniline (II) [13311-84-7] was prepared by treating 4-nitro-3-trifluoromethylaniline [393-11-3] with isobutyryl chloride [79-30-1]. Tablets were prepared by combining II 5, starch 5, lactose 89.5, and Mg stearate 0.5 mg/tablet.

IT 39240-77-2P

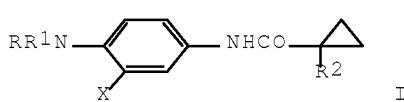
10/560012

RL: PREP (Preparation)  
(preparation of, as testosterone inhibitor)  
RN 39240-77-2 ZCPLUS  
CN Butanamide, 2,3-dimethyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 35 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1980:58461 ZCPLUS Full-text  
DOCUMENT NUMBER: 92:58461  
ORIGINAL REFERENCE NO.: 92:9675a, 9678a  
TITLE: Cycloalkanecarboxanilide derivative herbicides  
INVENTOR(S): Pilgram, Kurt H. G.; Skiles, Richard D.  
PATENT ASSIGNEE(S): Shell Oil Co., USA  
SOURCE: U.S., 5 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 7  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4168153	A	19790918	US 1978-876594	19780210 <--
CA 1087186	A1	19801007	CA 1978-294281	19780104 <--
BE 863074	A1	19780719	BE 1978-184445	19780119 <--
SE 7800692	A	19780722	SE 1978-692	19780119 <--
NL 7800656	A	19780725	NL 1978-656	19780119 <--
DE 2802282	A1	19780727	DE 1978-2802282	19780119 <--
JP 53092739	A	19780815	JP 1978-3778	19780119 <--
BR 7800354	A	19781010	BR 1978-354	19780119 <--
AU 7832543	A	19790726	AU 1978-32543	19780119 <--
AU 523765	B2	19820812		
AT 7800395	A	19800615	AT 1978-395	19780119 <--
AT 360799	B	19810126		
GB 1593932	A	19810722	GB 1978-2214	19780119 <--
CH 637917	A5	19830831	CH 1978-563	19780119 <--
PRIORITY APPLN. INFO.:			US 1977-761515	A2 19770121 <--
GI				

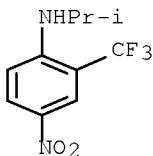


AB Seventeen cyclopropanecarboxanilides I ( $R = H, Me, Pr; R1 = H, Me, Me2CH, Me3C$ , cyclopropyl, 1-methylcyclopropyl, Pr;  $R2 = Me, Cl, Et; X = CF3, NO2, Br, Me$ ) were prepared by acylation of the appropriate aniline with a cyclopropanecarbonyl chloride. Tests with 15 I showed both pre- and postemergence herbicidal activity. Thus, acylation of 4,3-(Me<sub>2</sub>CHNH)(F<sub>3</sub>C)C<sub>6</sub>H<sub>3</sub>NH<sub>2</sub> with 1-methylcyclopropanecarbonyl chloride gave 84% I ( $R = H, R1 = Me2CH, R2 = Me, X = CF3$ ).

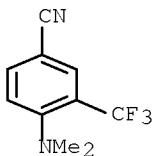
IT 70339-08-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and reduction of nitro group in)

RN 70339-08-1 ZCPLUS

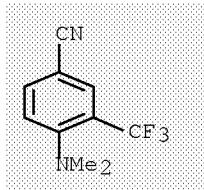
CN Benzenamine, N-(1-methylethyl)-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 36 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1979:523221 ZCPLUS Full-text  
 DOCUMENT NUMBER: 91:123221  
 ORIGINAL REFERENCE NO.: 91:19879a,19882a  
 TITLE: Dipole moment study of the ortho-effect in  
 4-substituted NN-dimethyl-2-trifluoromethylanilines  
 Hallas, Geoffrey; Hepworth, John D.; Jones, Peter;  
 Ibbetson, Douglas A.; Jones, Alan M.; Turton, Andrew  
 R.  
 CORPORATE SOURCE: Dep. Colour Chem., Leeds Univ., Leeds, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions  
 2: Physical Organic Chemistry (1972-1999) (1979),  
 (4), 525-8  
 CODEN: JCPKBH; ISSN: 0300-9580  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Apparent dipole moments of 4,2-R(CF<sub>3</sub>)C<sub>6</sub>H<sub>3</sub>NMe<sub>2</sub> ( $R = H, Me, Cl, Br, iodo, cyano, O2N, Me2N, H2N$ ) in C<sub>6</sub>H<sub>6</sub> were determined. Vector moments in the direction of the major axis of the ring were calculated to explain the observed dipole moments. These vector moments are compared with corresponding values calculated for 4-RC<sub>6</sub>H<sub>4</sub>NMe<sub>2</sub> ( $R = Cl, Br, iodo, cyano, O2N$ ). The influence of the 2-CF<sub>3</sub> group on the extent to which para substitution restores conjugation between the Me<sub>2</sub>N group and the ring is noted.  
 IT 71145-96-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and ortho effect in, dipole moment study of)  
 RN 71145-96-5 ZCPLUS  
 CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



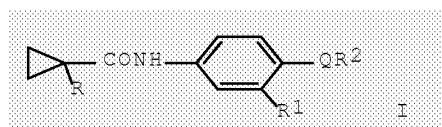
L70 ANSWER 37 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1979:490927 ZCPLUS Full-text  
 DOCUMENT NUMBER: 91:90927  
 ORIGINAL REFERENCE NO.: 91:14683a,14686a  
 TITLE: Evidence for electronic buttressing in 4-substituted NN-dimethyl-2-trifluoromethylanilines: long range fluorine-19-proton coupling  
 AUTHOR(S): Bartle, Keith D.; Hallas, Geoffrey; Hepworth, John D.; Jones, Peter; Matthews, Raymond S.  
 CORPORATE SOURCE: Dep. Phys. Chem., Univ. Leeds, Leeds, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1979), (2), 192-4  
 CODEN: JCPKBH; ISSN: 0300-9580  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The 1H NMR spectra of fourteen 4,2-R(F3C)C6H4NMe2 were examined. A long range 19F-1H coupling 6J(F,H) between NMe and CF3 was confirmed by 19F NMR. A linear relation holds between 6J(F,H) in these compds. and the appropriate Hammett para substituent consts. in accord with the operation of electronic buttressing; a similar correlation holds between the chemical shift of the N-Me protons and  $\sigma_p$ .  
 IT 71145-96-5  
 RL: PRP (Properties)  
 (NMR of, electronic buttressing in relation to)  
 RN 71145-96-5 ZCPLUS  
 CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 38 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1979:203718 ZCPLUS Full-text  
 DOCUMENT NUMBER: 90:203718  
 ORIGINAL REFERENCE NO.: 90:32397a,32400a  
 TITLE: Cycloalkanecarboxanilides with herbicide activity  
 INVENTOR(S): Pilgram, Kurt H. G.; Skiles, Richard D.  
 PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V., Neth.  
 SOURCE: Fr. Demande, 57 pp.  
 CODEN: FRXXBL

DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 7  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2377999	A1	19780818	FR 1978-1493	19780119 <--
FR 2377999	B1	19810327		
CA 1087186	A1	19801007	CA 1978-294281	19780104 <--
BE 863074	A1	19780719	BE 1978-184445	19780119 <--
SE 7800692	A	19780722	SE 1978-692	19780119 <--
NL 7800656	A	19780725	NL 1978-656	19780119 <--
DE 2802282	A1	19780727	DE 1978-2802282	19780119 <--
JP 53092739	A	19780815	JP 1978-3778	19780119 <--
BR 7800354	A	19781010	BR 1978-354	19780119 <--
AU 7832543	A	19790726	AU 1978-32543	19780119 <--
AU 523765	B2	19820812		
AT 7800395	A	19800615	AT 1978-395	19780119 <--
AT 360799	B	19810126		
GB 1593932	A	19810722	GB 1978-2214	19780119 <--
CH 637917	A5	19830831	CH 1978-563	19780119 <--
PRIORITY APPLN. INFO.:			US 1977-761515	A 19770121 <--
GI				

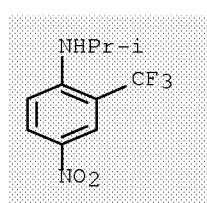


AB Ninety-four herbicidal I ( $R = C1-6$  alkyl, Cl, F, Br, alkoxy or alkylthio;  $R1 =$  halo, CN, NO<sub>2</sub>, CR<sub>3</sub>:NOR<sub>3</sub>, COR<sub>3</sub>, Q<sub>1</sub>R<sub>3</sub>;  $R2 =$  optionally halogenated alkyl, alkenyl or aryl, alkynyl, alkoxyalkyl, etc.;  $R3 = H$ , alkyl or cycloalkyl;  $Q = O, S, SO, SO_2$  or NR<sub>3</sub>;  $Q1 = O, S, SO$  or SO<sub>2</sub>) were prepared; extensive data for both pre- and postemergence application are given. Thus, 3,4-(F<sub>3</sub>C)C<sub>1</sub>C<sub>6</sub>H<sub>3</sub>NO<sub>2</sub> was treated with Me<sub>2</sub>CHONa, the NO<sub>2</sub> group was reduced, and the aniline was acylated with 1-methylcyclopropanecarbonyl chloride to give I ( $R = Me, R1 = C1, R2 = Me_2CH, Q = O$ ).

IT 70339-08-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reduction of)

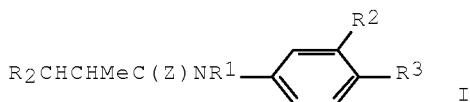
RN 70339-08-1 ZCAPLUS

CN Benzenamine, N-(1-methylethyl)-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 39 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1978:22155 ZCPLUS Full-text  
 DOCUMENT NUMBER: 88:22155  
 ORIGINAL REFERENCE NO.: 88:3549a, 3552a  
 TITLE: Alkanoic acid anilides  
 INVENTOR(S): Neri, Rudolph O.; Topliss, John G.  
 PATENT ASSIGNEE(S): Scherico Ltd., Switz.  
 SOURCE: Can., 56 pp.  
 CODEN: CAXXA4  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 1012462	A1	19770621	CA 1971-116108	19710618 <--
PRIORITY APPLN. INFO.:			CA 1971-116108	A 19710618 <--
GI				

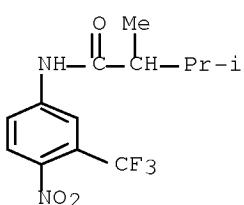


AB Eight alkanoic anilides I ( $Z = O, S$ ;  $R = H, Me$ ;  $R1 = H, Me, Et$ ;  $R2 = CF3, Cl, Br$ ;  $R3 = NO2, Cl$ ), which are useful as anti-androgenic agents (no data), were prepared by various methods. Amidation of  $Me_2CHCOCl$  by an aniline derivative yielded I ( $Z = O$ ,  $R = R1 = H$ ,  $R2 = CF3$ ,  $R3 = NO2$ ). The Beckmann rearrangement of  $4,3-Cl(F_3C)C_6H_3C(:NOH)CHMe_2$  gave I ( $R = R1 = H$ ,  $R2 = CF3$ ,  $R3 = Cl$ ,  $Z = O$ ). I ( $R = R1 = H$ ,  $R2 = CF3$ ,  $R3 = NO2$ ,  $Z = S$ ) was prepared from  $Me_2CHCS_2Me$  and the resp. aniline.

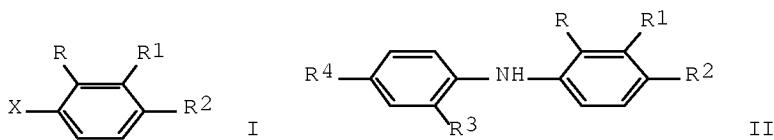
IT 39240-77-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 39240-77-2 ZCPLUS

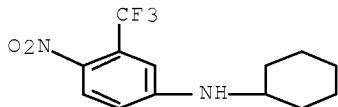
CN Butanamide, 2,3-dimethyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 40 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1977:189358 ZCPLUS Full-text  
DOCUMENT NUMBER: 86:189358  
ORIGINAL REFERENCE NO.: 86:29689a,29692a  
TITLE: Synthesis of 4-aminodiphenylamine and its relatives  
AUTHOR(S): Rondestvedt, Christian S., Jr.  
CORPORATE SOURCE: Jackson Lab., E. I. Du Pont de Nemours and Co.,  
Wilmington, DE, USA  
SOURCE: Journal of Organic Chemistry (1977), 42(10), 1786-90  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 86:189358  
GI

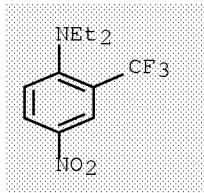


AB Formanilides and acetanilides condensed with halonitrobenzenes I ( $R = NO_2, H, Cl; R_2 = H, CF_3; R_3 = H, Me, NO_2; X = Cl, F$ ) to give eight resp. diphenylamines II ( $R_3 = H, Me; R_4 = H, OEt$ ).  
 IT 61587-18-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
     (preparation of)  
 RN 61587-18-6 ZCAPLUS  
 CN Benzenamine, N-cyclohexyl-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 41 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1975:409343 ZCPLUS Full-text  
DOCUMENT NUMBER: 83:9343  
ORIGINAL REFERENCE NO.: 83:1545a,1548a  
TITLE: Substituted N,N-dimethylanilines containing an o-trifluoromethyl group. Synthesis of N,N-dimethyl-2-trifluoromethylaniline  
AUTHOR(S): Hepworth, John D.; Jones, Peter; Hallas, Geoffrey  
CORPORATE SOURCE: Div. Chem., Polytech. Preston, Preston, UK  
SOURCE: Synthesis (1974), (12), 874-6  
CODEN: SYNTBF; ISSN: 0039-7881  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 83:9343

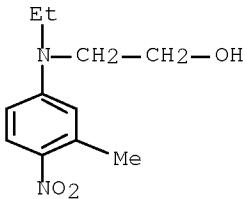
GI For diagram(s), see printed CA Issue.  
 AB The amines I ( $X = \text{Me}_2\text{N}$ ,  $\text{MeNH}$ , piperidino, morpholino,  $\text{Et}_2\text{N}$ ) were prepared in 74–94% yield by the reaction of I ( $X = \text{Cl}$ ) with the corresponding amine. Reduction of I ( $X = \text{Me}_2\text{N}$ ) gave 94%  $4,2-\text{H}_2\text{N}(\text{F}_3\text{C})\text{C}_6\text{H}_3\text{NMe}_2$  (II), which was converted to its Ac and Bz derivs. Diazotization of II followed by treatment with  $\text{CuBr}$  in  $\text{HBr}$  gave 91%  $4,2-\text{Br}(\text{F}_3\text{C})\text{C}_6\text{H}_3\text{NMe}_2$ , which when treated with  $\text{BuLi}$  gave 72%  $2-\text{F}_3\text{CC}_6\text{H}_4\text{NMe}_2$ .  
 IT 25900-35-0  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 25900-35-0 ZCPLUS  
 CN Benzenamine, N,N-diethyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 42 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1974:425336 ZCPLUS Full-text  
 DOCUMENT NUMBER: 81:25336  
 ORIGINAL REFERENCE NO.: 81:4085a, 4088a  
 TITLE: p-Nitroaniline derivatives  
 INVENTOR(S): Suda, Hideaki; Kanda, Tatsuo; Tomita, Hiroshige;  
 Nakanishi, Hirotoshi; Hida, Hiroshi; Nuno, Tatsumi  
 SUMITOMO Chemical Co., Ltd.  
 PATENT ASSIGNEE(S):  
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 5  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 49020129	A	19740222	JP 1972-63507	19720623 <--
CA 1012553	A1	19770621	CA 1973-174587	19730621 <--
DE 2331900	A1	19740124	DE 1973-2331900	19730622 <--
DE 2331900	C2	19861113		
FR 2199533	A1	19740412	FR 1973-22956	19730622 <--
IT 991637	B	19750830	IT 1973-68879	19730622 <--
GB 1421600	A	19760121	GB 1973-29902	19730622 <--
CH 593236	A5	19771130	CH 1973-9211	19730625 <--
FR 2225423	A1	19741108	FR 1974-3932	19740206 <--
FR 2225423	B1	19780616		
PRIORITY APPLN. INFO.:			JP 1972-18191	A 19720213 <--
			JP 1972-63507	A 19720623 <--
			JP 1972-63508	A 19720623 <--
			JP 1972-63509	A 19720623 <--
			JP 1972-63512	A 19720623 <--
			JP 1972-63513	A 19720623 <--
			JP 1972-64714	A 19720627 <--
			JP 1972-66286	A 19720701 <--
			JP 1973-18191	A 19730213 <--

- GI For diagram(s), see printed CA Issue.
- AB The nitroanilines (I; R<sub>1</sub>, R<sub>2</sub> = H, C<sub>1</sub>-6alkyl, CH<sub>2</sub>CH<sub>2</sub>OH, CH<sub>2</sub>CH<sub>2</sub>Cl, β-acylaminoethyl, CH<sub>2</sub>CH<sub>2</sub>NHSO<sub>2</sub>Me, but not R<sub>1</sub> = R<sub>2</sub> = H) were prepared by treating the nitrophenol ethers (II; R<sub>3</sub> = C<sub>1</sub>-6 alkyl, Ph) with HNR<sub>1</sub>R<sub>2</sub>. Thus, heating II (R<sub>3</sub> = Me) with 15 mole 20% aqueous EtNH<sub>2</sub> at 180° for 10 hr gave 97% I (R<sub>1</sub> = Et, R<sub>2</sub> = H) with 93% conversion. Among 5 more I prepared were the following (R<sub>1</sub>, R<sub>2</sub> given): Pr, H; CH<sub>2</sub>CH<sub>2</sub>OH, H; CH<sub>2</sub>CH<sub>2</sub>OH, Et; CH<sub>2</sub>CH<sub>2</sub>NHSO<sub>2</sub>Me, Et.
- IT 52177-13-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)
- RN 52177-13-6 ZCPLUS
- CN Ethanol, 2-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



L70 ANSWER 43 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1974:108165 ZCPLUS Full-text  
 DOCUMENT NUMBER: 80:108165  
 ORIGINAL REFERENCE NO.: 80:17387a,17390a  
 TITLE: N,N-Disubstituted p-phenylenediamines  
 INVENTOR(S): Suda, Hideaki; Kanda, Tatsuo; Tomita, Hiroshige;  
 Nakanishi, Hirotoshi; Hida, Himoru; Nuno, Tatsushi  
 SUMITOMO Chemical Co., Ltd.  
 PATENT ASSIGNEE(S):  
 SOURCE: Ger. Offen., 53 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 5  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2331900	A1	19740124	DE 1973-2331900	19730622 <--
DE 2331900	C2	19861113		
JP 49020129	A	19740222	JP 1972-63507	19720623 <--
JP 49020130	A	19740222	JP 1972-63508	19720623 <--
JP 51024491	B	19760724		
JP 49020131	A	19740222	JP 1972-63512	19720623 <--
JP 51040061	B	19761101		
JP 49020128	A	19740222	JP 1972-63513	19720623 <--
JP 55008501	B	19800304	JP 1972-63509	19720623 <--
JP 49020133	A	19740222		
JP 49024924	A	19740305	JP 1972-64714	19720627 <--
JP 55010577	B	19800317		
JP 49024923	A	19740305	JP 1972-66286	19720701 <--
JP 49102629	A	19740927	JP 1973-18191	19730213 <--
JP 52005486	B	19770214		
US 3920739	A	19751118	US 1973-378059	19730711 <--

10/560012

PRIORITY APPLN. INFO.:

JP 1972-63507	A 19720623 <--
JP 1972-63508	A 19720623 <--
JP 1972-63509	A 19720623 <--
JP 1972-63512	A 19720623 <--
JP 1972-63513	A 19720623 <--
JP 1972-64714	A 19720627 <--
JP 1972-66286	A 19720701 <--
JP 1973-18191	A 19730213 <--

GI For diagram(s), see printed CA Issue.

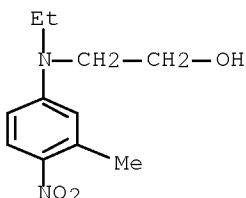
AB Four diamines I (R = H, Me; R1 = Et, CH<sub>2</sub>CH<sub>2</sub>OMe, CH<sub>2</sub>CH<sub>2</sub>NHSO<sub>2</sub>Me) were prepared in ≤100% yield by alkylation of II and subsequent reaction with R1NHET or successively with EtNH<sub>2</sub> and R1X(X = Cl, OH), or with EtNH<sub>2</sub>, ClSO<sub>2</sub>Me, and HOCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> followed by reduction over Pd/C.

IT 52177-13-6P 52177-25-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

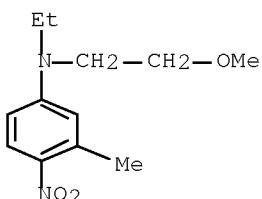
RN 52177-13-6 ZCPLUS

CN Ethanol, 2-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



RN 52177-25-0 ZCPLUS

CN Benzenamine, N-ethyl-N-(2-methoxyethyl)-3-methyl-4-nitro- (CA INDEX NAME)



L70 ANSWER 44 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1974:61050 ZCPLUS Full-text

DOCUMENT NUMBER: 80:61050

ORIGINAL REFERENCE NO.: 80:9905a,9908a

TITLE: Steric effects in di- and triarylmethane dyes. XI. Electronic absorption spectra of derivatives of Michler's hydrol blue, crystal violet, and malachite green containing o-trifluoromethyl groups

AUTHOR(S): Grocock, D. E.; Hallas, G.; Hepworth, J. D.

CORPORATE SOURCE: Dep. Sci., North Lindsay Coll. Technol., Scunthorpe, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions

2: Physical Organic Chemistry (1972-1999) (1973),  
 (13), 1792-6  
 CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal  
 LANGUAGE: English

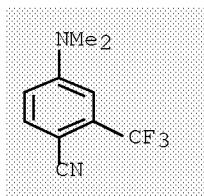
AB The effects of substitution of o-CF<sub>3</sub> groups in Michler's hydrol blue [14844-71-4], crystal violet [548-62-9], and malachite green [569-64-2] were examined. Bathochromic shifts of the first bands were observed for electronically sym. dyes. Addition of a CF<sub>3</sub> group at the 2'-position of malachite green produced a conformational change which caused a hypsochromic shift of the first band. In certain cases, the combined steric and electronic effects of the CF<sub>3</sub> groups were enough to shift the equilibrium between dye base and univalent dye cation in acid solution in favor of the former species.

IT 51332-25-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 51332-25-3 ZCPLUS

CN Benzonitrile, 4-(dimethylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 45 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1973:478429 ZCPLUS Full-text

DOCUMENT NUMBER: 79:78429

ORIGINAL REFERENCE NO.: 79:12713a,12716a

TITLE: Antiandrogenic substituted anilides

PATENT ASSIGNEE(S): Scherico Ltd.

SOURCE: Fr. Demande, 40 pp.

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2142803	A1	19730202	FR 1971-23250	19710625 <--
FR 2142803	B1	19740830		

PRIORITY APPLN. INFO.: FR 1971-23250 A 19710625 <--

GI For diagram(s), see printed CA Issue.

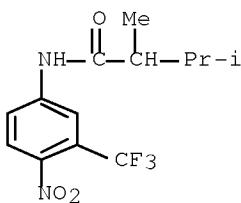
AB Ten anilides (I; R = CHMe<sub>2</sub>, CHMeCHMe<sub>2</sub>; R<sub>1</sub> = H, Me, Et; R<sub>2</sub> = CF<sub>3</sub>, SOCF<sub>3</sub>, Br, Cl; R<sub>3</sub> = NO<sub>2</sub>, Cl), potential antiandrogenic agents, are prepared by thirteen standard methods.

IT 39240-77-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

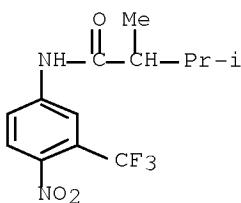
RN 39240-77-2 ZCPLUS

CN Butanamide, 2,3-dimethyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 46 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1973:58091 ZCPLUS Full-text  
 DOCUMENT NUMBER: 78:58091  
 ORIGINAL REFERENCE NO.: 78:9207a,9210a  
 TITLE: Substituted anilides and thioanilides  
 INVENTOR(S): Neri, Rudolph O.; Topliss, John G.  
 PATENT ASSIGNEE(S): Scherico Ltd.  
 SOURCE: Ger. Offen., 73 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

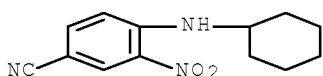
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2130450	A	19721221	DE 1971-2130450	19710619 <--
DE 2130450	B2	19771013		
JP 56049884	B	19811125	JP 1971-45301	19710624 <--
PRIORITY APPLN. INFO.:			DE 1971-2130450	A 19710619 <--
AB	Nine anilides 3,4-RR1C6H3NR2CXR3 (I; R = Cl, F3C, F3CSO; R1 = Cl, O2N; R2 = H, Me, Et; R3 = CHMe2, CHMeCHMe2; X = O, S), useful antiandrogenic agents, were prepared mainly by acylation of 3,4-RR1C6H3NH2 (II). Thus, Me2CHCOCl was heated with II (R = F3C, R1 = O2N) in pyridine for 1.5 hr to give I (R = F3C, R1 = O2N, R2 = H, R3 = CHMe2, X = O).			
IT	39240-77-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
RN	39240-77-2 ZCPLUS			
CN	Butanamide, 2,3-dimethyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)			



L70 ANSWER 47 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1970:121102 ZCPLUS Full-text

10/560012

DOCUMENT NUMBER: 72:121102  
ORIGINAL REFERENCE NO.: 72:21755a, 21758a  
TITLE: Antitubercular substances. XXI. Synthesis of 2-nitrodiphenylamines  
AUTHOR(S): Belton, J. G.; McInerney, Mary  
CORPORATE SOURCE: Lab. Med. Res. Counc. Ireland, Trinity Coll., Dublin, Ire.  
SOURCE: Proceedings of the Royal Irish Academy, Section B: Biological, Geological and Chemical Science (1970), 69(2), 21-9  
CODEN: PRIBAN; ISSN: 0035-8983  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI For diagram(s), see printed CA Issue.  
AB The title compds. (I) were prepared by heating halonitrobenzenes with anilines or cyclohexylamine, by treating nitroanilines with halobenzenes in the presence of anhydrous K<sub>2</sub>CO<sub>3</sub>, KIO<sub>4</sub>, and reduced Cu, by treating dinitrobenzenes with haloanilines, or by replacing Cl with alkoxy, thioalkyl, or amido groups on a preformed diphenylamine. The following (I) were prepared (R<sub>1</sub>, R<sub>2</sub>, R, m.p., and % yield given): CN, H, Ph, 126° (alc.), -; F<sub>3</sub>C, H, C<sub>6</sub>H<sub>11</sub>, 80-1° (light petroleum), 75; F<sub>3</sub>C, H, Ph, 84-5° (alc.), 69; Et, H, Ph, 121° (MeOH), -; HO<sub>2</sub>C, H, Ph, 220° (alc.), -; Cl, H, Ph, 61° (alc.), -; Cl, Cl, Ph, 96°, 61; H, H, 4-C<sub>1</sub>C<sub>6</sub>H<sub>4</sub>, 150°, 25; Cl, H, 3-MeOC<sub>6</sub>H<sub>4</sub>, 92-3°, 60; Cl, H, 4-MeOC<sub>6</sub>H<sub>4</sub>, 121°, 70; Cl, H, 3-EtOC<sub>6</sub>H<sub>4</sub>, 92°, 68; Cl, H, 4-EtOC<sub>6</sub>H<sub>4</sub>, 95°, 80; F, H, Ph, 53°, -; H, H, 3-MeOC<sub>6</sub>H<sub>4</sub>, 57-8° (alc.), 44; H, H, 4-MeOC<sub>6</sub>H<sub>4</sub>, 89°, 50; H, H, 3-EtOC<sub>6</sub>H<sub>4</sub>, 47.5-8.5° (alc.), 30; H, H, 4-EtOC<sub>6</sub>H<sub>4</sub>, 84°, 56; tert-Bu, H, Ph, 73-4° (alc.), -; EtO, H, Ph, 74°, 52; BuO, H, Ph, 57-8° (alc.), 40; EtO, H, 4-C<sub>1</sub>C<sub>6</sub>H<sub>4</sub>, 68-9° (alc.), -; Cl, H, 4-MeOC<sub>6</sub>H<sub>4</sub>, 112-14° (alc.) 40; MeO, H, 4-MeC<sub>6</sub>H<sub>4</sub>, 85-6° (alc.), 50; EtO, H, 4-MeC<sub>6</sub>H<sub>4</sub>, 75° (alc.), 50; H, H, 3-MeC<sub>6</sub>H<sub>4</sub>, 70-1° (MeOH), 71; H, Cl, 4-BrC<sub>6</sub>H<sub>4</sub>, 160-1° (C<sub>6</sub>H<sub>6</sub>-alc.), -; H, Cl, 3-C<sub>1</sub>C<sub>6</sub>H<sub>4</sub>, 109° (alc.), 30; H, Cl, 4-IC<sub>6</sub>H<sub>4</sub>, 186-7°, -; H, MeO, 4-BrC<sub>6</sub>H<sub>4</sub>, 149° (alc.), -; H, MeO, 4-IC<sub>6</sub>H<sub>4</sub>, 167° (alc.), 80-90; H, MeO, 3-C<sub>1</sub>C<sub>6</sub>H<sub>4</sub>, 107° (alc.), 80-90; Cl, MeO, Ph, 103-4° (alc.), 80-90; H, MeO, C<sub>6</sub>H<sub>11</sub>, 78-9° (alc.), 80-90; H, EtO, Ph, 107-8° (alc.), -; H, MeS, 4-C<sub>1</sub>C<sub>6</sub>H<sub>4</sub> (II), 133° (alc.), -; H, MeS, Ph, 135° (alc.), -; H, phthalimido, Ph, 203-4°, -; H, NH<sub>2</sub>, Ph, 126-7° (aqueous alc.), -; H, NHAc, Ph, 202-3°, -; Cl, C<sub>6</sub>H<sub>11</sub>, Ph, 124-5° (light petroleum), -. Na<sub>2</sub>S<sub>2</sub>.9H<sub>2</sub>O, and S in 95% aqueous alc. were added to 5,4'-dichloro-2-nitrodiphenylamine in 95% aqueous alc. and HCONMe<sub>2</sub> and heated on a water bath 2 hr to give 3,3'-bis(p-chloroanilino)-4,4'-dinitrophenyl disulfide, yellow, m. 190-1° (HCONMe<sub>2</sub>-alc.), which was used to prepare II.  
IT 28096-55-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
RN 28096-55-1 ZCAPLUS  
CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)

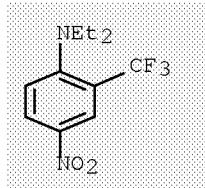


L70 ANSWER 48 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1970:66670 ZCAPLUS Full-text  
DOCUMENT NUMBER: 72:66670

10/560012

ORIGINAL REFERENCE NO.: 72:12151a,12154a  
TITLE: Herbicidal alkylaminophenylureas  
INVENTOR(S): Schwartz, Herbert; Skaptason, Joseph B.  
SOURCE: U.S., 4 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3484484	A	19691216	US 1967-626409	19670328 <--
PRIORITY APPLN. INFO.:			US 1967-626409	A 19670328 <--
GI	For diagram(s), see printed CA Issue.			
AB	The title compounds (I) are useful as preemergent and postemergent herbicides. Thus, a mixture of 98 g 4-chloro-3-(trifluoromethyl)-nitrobenzene and 97 g Pr <sub>2</sub> NH in 150 ml MeOH was refluxed overnight to give 89 g II (R <sub>1</sub> = R <sub>2</sub> = Pr, X = CF <sub>3</sub> , Y = NO <sub>2</sub> ), b0.5 86-9°, which was hydrogenated over Pd/C to give II (R <sub>1</sub> = R <sub>2</sub> = Pr, X = NH <sub>2</sub> ), b1 85-8°, of which 14 g was dissolved in 150 ml C <sub>6</sub> H <sub>6</sub> , and 4.5 ml pyridine then 6 g Me <sub>2</sub> NCOCl added at room temperature to give I (R <sub>1</sub> = R <sub>2</sub> = Pr, X = CF <sub>3</sub> , R <sub>3</sub> = Me), m. 124-5° (C <sub>6</sub> H <sub>6</sub> -C <sub>6</sub> H <sub>14</sub> ). Similarly prepared were the tabulated I. Similarly prepared were II (R <sub>1</sub> = R <sub>2</sub> = Et, X = CF <sub>3</sub> , Y = NO <sub>2</sub> ), b1 95-8°, and II (R <sub>1</sub> = R <sub>2</sub> = Pr, X = Cl, Y = NO <sub>2</sub> ), m. 141-3°.			
IT	25900-35-Q8			
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
RN	25900-35-0 ZCAPLUS			
CN	Benzenamine, N,N-diethyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)			



L70 ANSWER 49 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1969:87264 ZCAPLUS Full-text  
DOCUMENT NUMBER: 70:87264  
ORIGINAL REFERENCE NO.: 70:16285a,16288a  
TITLE: Nitro(trifluoromethyl)toluidides  
INVENTOR(S): Baker, Joseph W.  
PATENT ASSIGNEE(S): Monsanto Co.  
SOURCE: U.S., 5 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3426049	A	19690204	US 1965-497437	19651018 <--
PRIORITY APPLN. INFO.:			US 1965-497437	A 19651018 <--

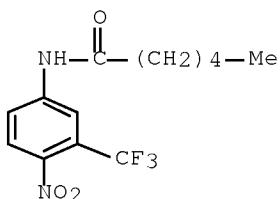
AB The title compds. possessing useful microbiol. activity were prepared Thus, 0.055 mole valeryl chloride was added to 0.05 mole  $\alpha,\alpha,\alpha$ -trifluoro-4-nitro-m-toluidine (I). The mixture was refluxed until the evolution of HCl ceased, 75 ml. methylcyclohexane added, and the mixture cooled to yield  $\alpha,\alpha,\alpha$ -trifluoro-4'-nitro-m-valerotoluidide (IIa), m. 94-5°. Similarly prepared were RCONHC<sub>6</sub>H<sub>3</sub>(CF<sub>3</sub>)NO<sub>2</sub>-3,4 (RCO and m.p. given): isovaleryl, (IIb), 103-4°; 2-methylbutyryl, 111-12°; 4-methylvaleryl, 85-7°; hexanoyl (IIc), 73-4°; neoheptanoyl, 110.5-12°; decanoyl, 77-8°; undecanoyl, 82-3°; cyclopentanecarbonyl, 143-4°; cyclohexanecarbonyl, 135-6°; hydrocinnamoyl, 90.5-92°; sorboyl, 123-4°; 3-ethyl-2-hexanoyl, 90-1°; 2-nonenoyl, 59-60°; 2-bromononanoyl, 102-3°; 2-chlorononanoyl, 55-6°; nonanoyl (II), 69-70°; heptanoyl (III), 64-5°; octanoyl (IV), 72-3°; lauroyl, 78-9°; 10-undecenoyl, 77-8°; 2-nonynoyl, 47-8°. A solution of 0.05 mole nonanoyl chloride in 25 ml. ether was added to a solution of 0.05 mole I and 0.05 mole Et<sub>3</sub>N in 200 ml. ether. The mixture was refluxed for 3 hrs., cooled, and Et<sub>3</sub>N-HCl removed to yield II-I complex, m. 84-5°. An excess of ethereal HCl was added to a solution of 10 g. II-I complex in 75 ml. ether and the toluidine-HCl removed to yield II. Similarly prepared were  $\alpha,\alpha,\alpha$ -trifluoro-4-methyl-4'-nitro-m-valerotoluidide-I complex, m. 97-8°; III-I complex, m. 94-5°; IV-I complex, m. 90-1°. A solution of 0.0017 mole IIa and 0.0017 mole I in 10 ml. toluene-methylcyclohexane mixture was cooled to give IIa-I complex, m. 96-7°. Similarly prepared were IIb-I complex, m. 103-4°; IIc-I complex, m. 106-7°. A solution of 0.014 mole Br in 25 ml. CCl<sub>4</sub> was added to a solution of 0.014 mole  $\alpha,\alpha,\alpha$ -trifluoro-4'-nitro-m-(2-nonenoyl)toluidide in 100 ml. CCl<sub>4</sub> at 0-5°, the mixture kept 6 hrs. at 0-5°, 1.5 g. KOAc in 10 ml. EtOH added, and the mixture refluxed 30 min. to give 2,3-dibromo- $\alpha,\alpha,\alpha$ -trifluoro-4'-nitro-m-nonanotoluidide, m. 107-8°.

IT 10023-90-2P 10023-91-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

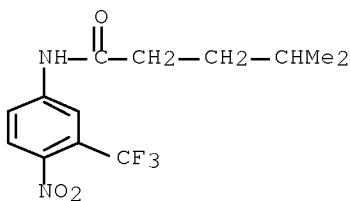
RN 10023-90-2 ZCPLUS

CN Hexanamide, N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 10023-91-3 ZCPLUS

CN Pentanamide, 4-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 50 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:37593 ZCPLUS Full-text

DOCUMENT NUMBER: 66:37593

ORIGINAL REFERENCE NO.: 66:7131a, 7134a

TITLE: Synthesis and bacteriostatic activity of some nitrotrifluoromethylanilides

AUTHOR(S): Baker, Joseph Willard; Bachman, Gerald L.; Schumacher, Ignatius; Roman, Daniel P.; Tharp, Alan L.

CORPORATE SOURCE: Org. Chems. Div., Monsanto Co., St. Louis, MO, USA

SOURCE: Journal of Medicinal Chemistry (1967), 10(1), 93-5

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

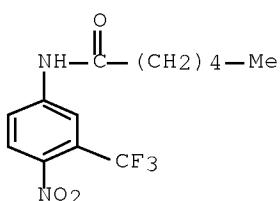
AB Nitrotrifluoromethylanilides (I) were prepared either by the acid-catalyzed reaction of an anhydride with a substituted aniline or by the condensation of an acid chloride or with the aniline alone or in the presence of Et<sub>3</sub>N as the HCl acceptor. Seven anilide-aniline complexes were formed when C5-9 acid chlorides free of  $\alpha$ -substituents were treated with 4-nitro-3-trifluoromethylaniline in the presence of Et<sub>3</sub>N. The active structures of the nitrotrifluoromethylanilides which inhibited the activity of *Staphylococcus aureus* included those which were substituted in the meta and para positions of the N-phenyl ring with a nitro and trifluoromethyl group and in which the acid-derived moiety incorporates alkyl, haloalkyl, cycloalkyl, alkenyl, haloalkenyl, alkylidенyl, and phenethyl groups and contains 5-12 C atoms. Anilides substituted in the  $\alpha$  position possessed a lower order of activity. Benzyl and phenoxy methyl derivs. and disubstituted and orthosubstituted derivs. were inactive. All of the complexes were derivs. of active anilides and exhibited the same order of activity on a weight basis as the anilides themselves.

IT 10023-90-2P 10023-91-3P

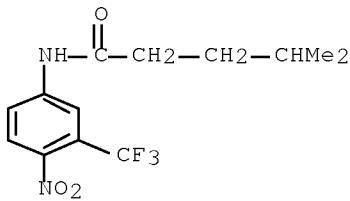
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 10023-90-2 ZCPLUS

CN Hexanamide, N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 10023-91-3 ZCPLUS  
 CN Pentanamide, 4-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 51 OF 51 ZCPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1942:29161 ZCPLUS Full-text

DOCUMENT NUMBER: 36:29161

ORIGINAL REFERENCE NO.: 36:4490c-f

TITLE: Alkanolamines. X. Intermediates of pentryl analogs.

Chloronitroanilinoalkanols

AUTHOR(S): Kremer, Chester B.; Meltsner, M.

SOURCE: Journal of the American Chemical Society (1942), 64, 1285-6

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 34, 6942.2. The condensations were carried out by refluxing for 4 h. the Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>NO<sub>2</sub> and twice the mol. quantity of the NH<sub>2</sub> alc. in BuOH. 2-(R-anilino)ethanols (R given): 4-chloro-2-nitro, m. 107.5°; 5-Cl isomer, m. 116°; 3-Cl isomer, m. 78.5°; 6-Cl isomer, b2 155-7°; 6-chloro-4-nitro, m. 120°. 3-(R-anilino)-1-propanols: 4-chloro-2-nitro, m. 60°; 5-Cl isomer, m. 78.5°; 6-chloro-4-nitro, m. 73°. 1-(R-anilino)-2-propanols: 4-chloro-2-nitro, m. 116.5°; 5-Cl isomer, m. 109°; 3-Cl isomer, m. 83.5°; 6-chloro-4-nitro, m. 144°. 1-(R-anilino)-2-methyl-2-propanols: 4-chloro-2-nitro, m. 121.5°; 5-Cl isomer, m. 127°; 3-Cl isomer, m. 98.5°; 6-chloro-4-nitro, m. 71.5°. 2-(4-Chloro-2-nitroanilino)-2-methyl-1-propanol, m. 122°. Reduction was effected with NaHSO<sub>3</sub> in a weakly alkaline medium: 2-(R-2-aminoanilino)ethanols: 4-Cl, m. 122.5°; 5-Cl, m. 104.5°; 3-Cl, m. 74°; 6-Cl, b2 135-7°. 3-(5-Chloro-2-aminoanilino)-1-propanol, m. 73.5°. 1-(4-Chloro-2-aminoanilino)-2-propanol, m. 130°; 5-Cl isomer, m. 101.5°. 1-(4-Chloro-2-aminoanilino)-2-methyl-2-propanol, m. 121°; 2-(4-chloro-2-aminoanilino)-2-methyl-1-propanol.

IT 854666-45-8P, 2-Propanol, 1-(2-chloro-4-nitroanilino)-2-methyl-

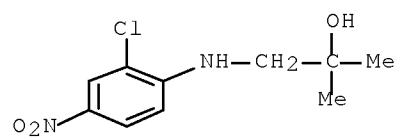
RL: PREP (Preparation)

(preparation of)

RN 854666-45-8 ZCPLUS

CN 2-Propanol, 1-[(2-chloro-4-nitrophenyl)amino]-2-methyl- (CA INDEX NAME)

10/560012



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(FILE 'HOME' ENTERED AT 08:38:37 ON 12 MAR 2009)

FILE 'REGISTRY' ENTERED AT 08:39:03 ON 12 MAR 2009

FILE 'ZCAPLUS' ENTERED AT 08:39:33 ON 12 MAR 2009

ACT BAS012APP/A

L1 1 SEA SPE=ON ABB=ON PLU=ON US2005-560012 /AP

FILE 'REGISTRY' ENTERED AT 08:39:39 ON 12 MAR 2009

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ACT BAS012HITRNS/A

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ACT BAS0120LDRNS/A

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L8 ( 1) SEA SPE=ON ABB=ON PLU=ON 115416-50-7  
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L10 6 SEA SPE=ON ABB=ON PLU=ON (L4 OR L5 OR L6 OR L7 OR L8 OR L9)

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D SCA

FILE 'STNGUIDE' ENTERED AT 08:41:38 ON 12 MAR 2009

FILE 'REGISTRY' ENTERED AT 08:45:14 ON 12 MAR 2009

L\*\*\* DEL 5594 S MG/ELS (P) BR/ELS  
L\*\*\* DEL 1 S ?GRIGNARD?/CNS  
D SCA

FILE 'STNGUIDE' ENTERED AT 08:51:02 ON 12 MAR 2009

FILE 'REGISTRY' ENTERED AT 09:22:39 ON 12 MAR 2009

D SCA L10  
L11 3 SEA SPE=ON ABB=ON PLU=ON L10 AND X/ELS

FILE 'ZCAPLUS' ENTERED AT 09:23:07 ON 12 MAR 2009

L12 12 SEA SPE=ON ABB=ON PLU=ON L11

FILE 'REGISTRY' ENTERED AT 09:23:40 ON 12 MAR 2009

L13 STRUCTURE UPLOADED  
L14 SCREEN 616  
L15 151 SEA SPE=ON ABB=ON PLU=ON L11 OR L3  
L16 0 SEA SPE=ON ABB=ON PLU=ON L15 AND C>21  
L17 SCREEN 1951  
L18 3 SEA SSS SAM L13 AND L14  
L19 6 SEA SSS SAM L13 AND (L14 NOT L17)  
D SCA

FILE 'STNGUIDE' ENTERED AT 09:31:23 ON 12 MAR 2009

10/560012

FILE 'REGISTRY' ENTERED AT 09:46:40 ON 12 MAR 2009  
D SCA L19

FILE 'STNGUIDE' ENTERED AT 09:52:26 ON 12 MAR 2009

FILE 'REGISTRY' ENTERED AT 10:01:51 ON 12 MAR 2009  
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L23 SCREEN 2043  
L24 SCREEN 2043 OR 1951  
L25 2 SEA SSS SAM L20 AND (L14 NOT L24)  
D SCA  
L26 STRUCTURE uploaded  
L27 SCREEN 1993  
L28 1 SEA SSS SAM L26 AND ((L14 AND L27) NOT L24)  
D SCA  
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D SCA  
L38 1054 SEA SUB=L35 SSS FUL L26 AND ((L14 AND L27) NOT L32)  
SAVE TEMP L38 BAS012STR26L/A

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FILE 'REGISTRY' ENTERED AT 10:26:04 ON 12 MAR 2009  
L40 1054 SEA SPE=ON ABB=ON PLU=ON L38 AND C<22  
L41 143 SEA SPE=ON ABB=ON PLU=ON L3 AND C>10  
L42 8 SEA SPE=ON ABB=ON PLU=ON L3 NOT L41  
D SCA  
L43 994 SEA SPE=ON ABB=ON PLU=ON L38 AND C>8

FILE 'ZCPLUS' ENTERED AT 10:28:08 ON 12 MAR 2009  
L44 2557 SEA SPE=ON ABB=ON PLU=ON L43

FILE 'REGISTRY' ENTERED AT 10:28:34 ON 12 MAR 2009  
L45 97 SEA SPE=ON ABB=ON PLU=ON L3 AND F/ELS  
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L47 135 SEA SPE=ON ABB=ON PLU=ON L38 AND L3  
L48 16 SEA SPE=ON ABB=ON PLU=ON L3 NOT L47  
D SCA  
L49 0 SEA SPE=ON ABB=ON PLU=ON L47 AND BR/ELS  
L50 1 SEA SPE=ON ABB=ON PLU=ON L48 AND BR/ELS AND 9/F  
D SCA

10/560012

L51 10 SEA SPE=ON ABB=ON PLU=ON L48 NOT BR/ELS  
D SCA  
L52 6 SEA SPE=ON ABB=ON PLU=ON L51 AND F/ELS  
L53 7 SEA SPE=ON ABB=ON PLU=ON L50 OR L52  
L54 142 SEA SPE=ON ABB=ON PLU=ON L47 OR L53  
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SEL MF  
D COST FULL  
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2/MF OR C10H11F3N2O2/MF OR C10H11F3N2O3/MF OR C10H13CLN2O3/MF  
OR C10H6F6N2/MF OR C10H9F3N2/MF OR C11H11F3N2/MF OR C11H11F3N2O  
/MF OR C11H13F3N2O2/MF OR C11H13F3N2O3/MF OR C11H13N3O3/MF OR  
C11H15CLN2O2/MF OR C11H16CLN3O2/MF OR C11H16N2O3/MF OR  
C11H7BRF9N/MF OR C12H10F6N2/MF OR C12H10F6N2O/MF OR C12H11F5N2/  
MF OR C12H11F6N3/MF OR C12H13F3N2O/MF OR C12H16CLN3/MF OR  
C12H18CLN3O2/MF OR C12H18N2O3/MF OR C12H7F9N2/MF OR C12H8F8N2/M  
F OR C12H9F6N5/MF OR C12H9F7N2/MF OR C13H12F6N2/MF OR C13H12F6N  
2O3S/MF OR C13H12F6N2S/MF OR C13H13CLN2/MF OR C13H13F3N2/MF OR  
C13H13F3N2O2/MF OR C13H13F6N3O2S/MF OR C13H15CLN2/MF OR  
C13H15F3N2O2/MF OR C13H15F3N2O3/MF OR C13H17CLN2O/MF OR  
C13H17F3N2O2/MF OR C13H17F3N2O3/MF OR C13H17F3N2O4/MF OR  
C13H18N2O3/MF OR C13H20N2O3/MF OR C13H8F6N2/MF OR C14H11F9N2O/M  
F OR C14H12F6N2/MF OR C14H13F3N2/MF OR C14H13F6N3O/MF OR  
C14H13F6N3O2/MF OR C14H14F6N2O/MF OR C14H15F3N2/MF OR C14H17CLN  
2/MF OR C14H17F3N2O/MF OR C14H17F3N2O3/MF OR C14H17N3/MF OR  
C14H19CLN2/MF OR C14H19F3N2O2/MF OR C14H20N2O2/MF OR C14H22N2O2  
/MF OR C15H14F6N2/MF OR C15H16F6N2/MF OR C15H17F3N2O2/MF OR  
C15H19N3O2/MF OR C15H21CLN2/MF OR C15H21CLN2O2/MF OR C15H21F3N2  
O2/MF OR C15H21N3O2/MF OR C15H24N2O2/MF OR C16H19F3N2/MF OR  
C16H19F3N2O2/MF OR C16H20F3NO/MF OR C16H21F3N2O/MF OR C16H21F3N  
2O2/MF OR C17H12F9N/MF OR C17H19F6N3O2/MF OR C17H23F3N2/MF OR  
C17H25N3O2/MF OR C18H27F3N4/MF OR C21H31F3N2OSI/MF OR C9H6F6N2O  
2/MF)  
L56 359 SEA SPE=ON ABB=ON PLU=ON L55 AND L38

FILE 'ZCAPLUS' ENTERED AT 10:56:37 ON 12 MAR 2009

L57 68 SEA SPE=ON ABB=ON PLU=ON L56  
L58 49 SEA SPE=ON ABB=ON PLU=ON L57 AND P/DT  
L59 19 SEA SPE=ON ABB=ON PLU=ON L57 NOT L58  
L60 16 SEA SPE=ON ABB=ON PLU=ON L59 AND PY<2004  
L61 28 SEA SPE=ON ABB=ON PLU=ON L58 AND PD<20030610  
L62 35 SEA SPE=ON ABB=ON PLU=ON L58 AND PRD<20030610  
L63 30 SEA SPE=ON ABB=ON PLU=ON L58 AND AD<20030610  
L64 51 SEA SPE=ON ABB=ON PLU=ON (L60 OR L61 OR L62 OR L63)  
D COST  
L65 1 SEA SPE=ON ABB=ON PLU=ON L54 AND L1

FILE 'REGISTRY' ENTERED AT 10:59:42 ON 12 MAR 2009

L66 142 SEA SPE=ON ABB=ON PLU=ON L55 AND L54  
L67 366 SEA SPE=ON ABB=ON PLU=ON L56 OR L66

FILE 'ZCAPLUS' ENTERED AT 11:00:41 ON 12 MAR 2009

10/560012

L68            68 SEA SPE=ON ABB=ON PLU=ON L67  
L69            1 SEA SPE=ON ABB=ON PLU=ON L68 AND L1  
L70            51 SEA SPE=ON ABB=ON PLU=ON L68 AND L64

FILE 'REGISTRY' ENTERED AT 11:02:00 ON 12 MAR 2009

FILE 'ZCPLUS' ENTERED AT 11:02:04 ON 12 MAR 2009  
D STAT QUE L69  
D IBIB ABS HITSTR L69 1

FILE 'REGISTRY' ENTERED AT 11:02:42 ON 12 MAR 2009  
D STAT QUE L70

FILE 'ZCPLUS' ENTERED AT 11:02:50 ON 12 MAR 2009  
D IBIB ABS HITSTR L70 1-51

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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FILE ZCPLUS

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FILE COVERS 1907 - 12 Mar 2009 VOL 150 ISS 11  
FILE LAST UPDATED: 11 Mar 2009 (20090311/ED)

ZCplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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10/560012

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

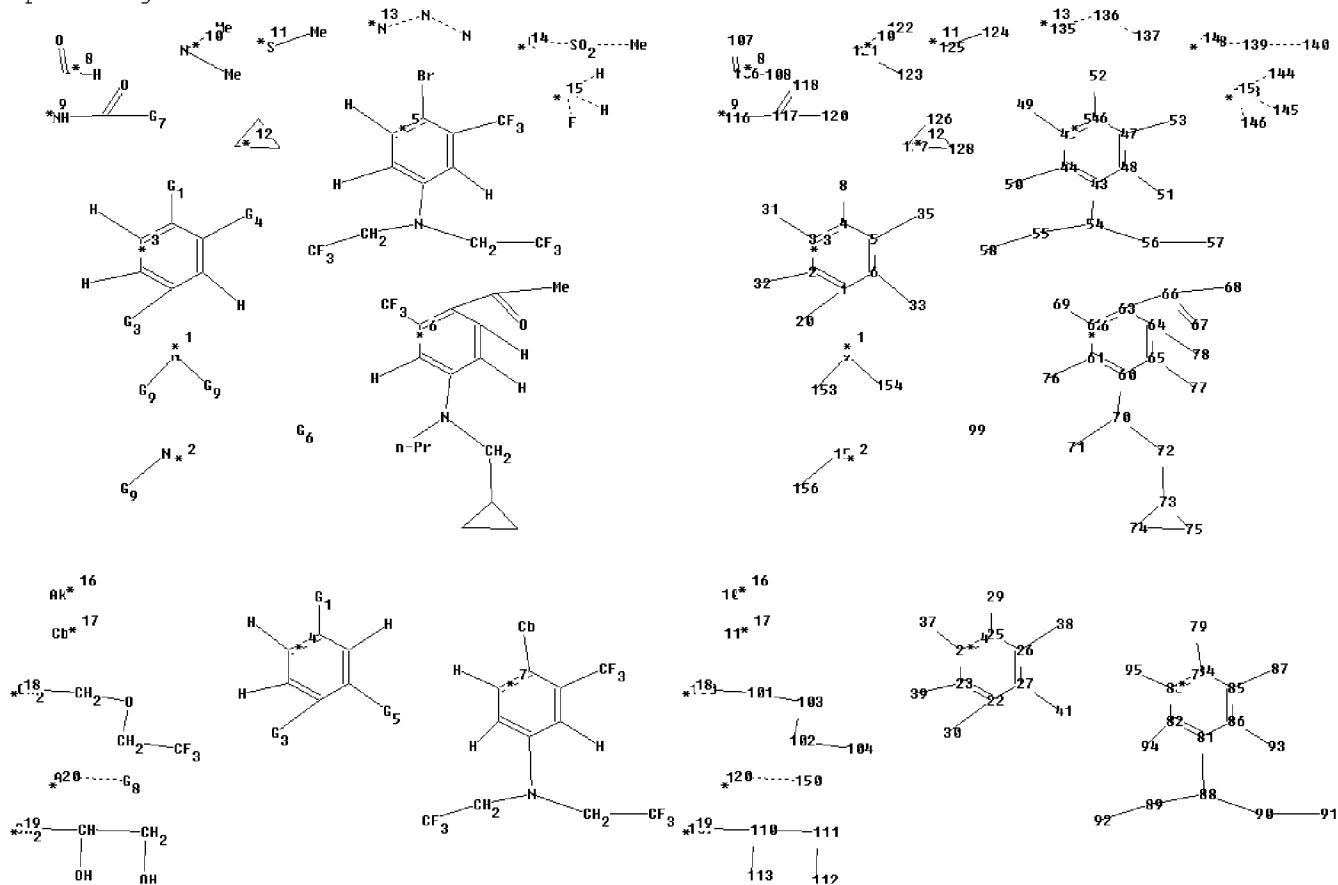
FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Mar 6, 2009 (20090306/UP).

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Uploading L26.str



10/560012

106-107 109-110  
110-111 110-113 111-112 115-150 116-117 117-118 117-120 121-122 121-123  
124-125 135-136  
136-137 138-139 139-140 143-144 143-145 143-146  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-48  
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 73-74 73-75  
74-75 81-82  
81-86 82-83 83-84 84-85 85-86 126-127 126-128 127-128  
exact/norm bonds :  
1-20 4-8 5-35 9-153 9-154 15-156 22-30 25-29 27-41 43-54 60-70 66-67  
73-74 73-75 74-75 81-88 106-107 110-113 115-150 116-117 117-118 117-120  
126-127 126-128  
127-128 135-136 136-137 138-139 139-140 143-144 143-145 143-146  
exact bonds :  
2-32 3-31 6-33 23-39 24-37 26-38 44-50 45-49 46-52 47-53 48-51 54-55  
54-56 55-58 56-57 61-76 62-69 63-66 64-78 65-77 66-68 70-71 70-72 72-73  
79-84 82-94 83-95  
85-87 86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-108 109-110  
110-111 111-112 121-122 121-123 124-125  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-48  
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 81-82 81-86  
82-83 83-84  
84-85 85-86  
isolated ring systems :  
containing 1 : 22 : 43 : 60 : 81 :

G1:CN,NO2

G3:[\*1],[\*2]

G4:CF3,Cl,NO2,CH3,OH,CN

G5:CH3,CF3,NO2,Cl

G6:[\*3],[\*4],[\*5],[\*6],[\*7]

G7:CH3,MeO,t-BuO

G8:CF3,OH,MeO,EtO,NH2,[\*8],[\*9],[\*10],[\*11],[\*12],[\*13],[\*14],[\*15]

G9:[\*16],[\*17],[\*18],[\*19],[\*20]

Hydrogen count :

9:= exact 0 15:= exact 1

Connectivity :

9:3 E exact RC ring/chain 10:1 E exact RC ring/chain 11:1 E exact RC ring/chain  
15:2 E exact RC ring/chain 79:1 E exact RC ring/chain 115:2 E exact RC ring/chain  
125:2 E exact  
RC ring/chain 126:2 E exact RC ring/chain 128:2 E exact RC ring/chain 138:2 E  
exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom  
15:CLASS 20:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 29:CLASS

10/560012

30:CLASS 31:CLASS  
32:CLASS 33:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 41:CLASS 43:Atom  
44:Atom 45:Atom  
46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS  
54:CLASS 55:CLASS  
56:CLASS 57:CLASS 58:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom  
66:CLASS  
67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:Atom 74:Atom  
75:Atom 76:CLASS 77:CLASS  
78:CLASS 79:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:CLASS  
88:CLASS  
89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 95:CLASS 99:CLASS  
100:CLASS 101:CLASS  
102:CLASS 103:CLASS 104:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS  
110:CLASS 111:CLASS  
112:CLASS 113:CLASS 115:CLASS 116:CLASS 117:CLASS 118:CLASS 120:CLASS  
121:CLASS 122:CLASS  
123:CLASS 124:CLASS 125:CLASS 126:Atom 127:Atom 128:Atom 135:CLASS 136:CLASS  
137:CLASS  
138:CLASS 139:CLASS 140:CLASS 143:CLASS 144:CLASS 145:CLASS 146:CLASS  
150:CLASS 153:CLASS  
154:CLASS 156:CLASS  
Generic attributes :  
11:  
Saturation : Saturated  
79:  
Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Type of Ring System : Monocyclic

Element Count :

Node 10: Limited  
C,C7

Node 11: Limited  
C,C6

Node 79: Limited  
C,C6

Node 115: Limited  
C,C6